Spectra data:

$[BrMg(\mu\text{-}O_2CPh)(THF)_2]_2$ (1). ^{1}H NMR [$(CD_3)_2SO$]: δ 1.73 (m, 8H, 3, 4 –thf –*H*), 3.57 (m, 8H, 2, 5 –thf –*H*), 7.38~7.41 (m, 3H, *m-H*/*p-H*), 8.05 (m, 2H, *o-H*). ^{13}C NMR [$(CD_3)_2SO$]: δ 25.18 (3, 4 –thf –*C*), 67.08 (2, 5 –thf –*C*), 127.76 (*m-C*), 129.82 (*o-C*), 131.03 (*p-C*), 135.67 (*ipso-C*), 172.25 (CO_2). Mass spectrum (EI: 70 eV) 10 most intense m/z: 42, 44, 78, 71, 72, 77, 69, 79, 105, 122. IR (KBr, cm^{-1}): 3069 s, 2889 s, 1626 br, 1573 s, 1494 s, 1428 s, 1314 s, 1176 s, 1035 s, 920 s, 880 s, 719 s, 673 s.

$[Mg_3(O_2C^iPr)_6(THF)_2]$ (2). ^{1}H NMR [$(CD_3)_2SO$]: δ 0.98 [d, 36H, $CH(CH_3)_2$], 1.76 (m, 8H, 3, 4 –thf –*H*), 2.26 [m, 6H, $CH(CH_3)_2$], 3.60 (m, 8H, 2, 5 –thf –*H*). ^{13}C NMR [$(CD_3)_2SO$]: δ 19.81 [$CH(CH_3)_2$], 25.12 (3, 4 –thf –*C*), 34.90 [$CH(CH_3)_2$], 67.02 (2, 5 –thf –*C*), 183.84 (CO_2). Mass spectrum (EI: 70 eV) 10 most intense m/z: 547, 549, 548, 230, 43, 231, 41, 550, 44, 551. IR (KBr, cm^{-1}): 2923 s, 2853 sh, 1582 m, 1457 s, 1372 m, 1295 w, 1169 w, 1100 w, 1073 w, 1038 w, 928 m, 891 w, 853 w, 787 w, 722 w, 673 w, 561 w.

$[Mg_3(O_2C^iPr)_6(HMPA)_2]$ (3). ^{1}H NMR (C_6D_6): δ 1.39 [d, 36H, $CH(CH_3)_2$], 2.39 [d, 36H, $(Me_2N)_3PO$], 2.84 [br, 6H, $CH(CH_3)_2$], ^{13}C NMR (C_6D_6): δ 20.72 [$CH(CH_3)_2$], 37.06 [$CH(CH_3)_2$], 37.11 [$(Me_2N)_3PO$], 185.42 (CO_2). ^{31}P NMR (C_6D_6): δ 24.09 [$(Me_2N)_3PO$]. Mass spectrum (EI: 70 eV) 10 most intense m/z: 135, 44, 179, 46, 180, 92, 136, 47, 93, 90. IR (KBr, cm^{-1}): 2966 s, 2923 sh, 2811 m, 1604 s, 1555 s, 1465 s, 1416 s, 1373 m, 1356 m, 1304 s, 1208 s, 1131 m, 1093 m, 1070 m, 991 s, 944 w, 928 w, 861 w, 837 w, 609 m, 531 w, 477 s, 420 s.

$[Mg_3(O_2CC{\equiv}CPh)_6(THF)_2]$ (4). ^{1}H NMR [$(CD_3)_2SO$]: δ 1.74 (m, 8H, 3, 4 –thf –*H*), 3.59 (m, 8H, 2, 5 –thf –*H*), 7.36~7.46 (m, 30H, C_6H_5), ^{13}C NMR [$(CD_3)_2SO$]: δ 25.15 (3, 4 –thf –*C*), 67.04 (2, 5 –thf –*C*), 76.21 (*C*≡CPh), 89.46 (C≡*C*Ph), 122.13 (*ipso-C*), 128.72 (*p-C*), 128.78 (*m-C*), 131.66 (*o-C*), 156.54 (CO_2). Mass spectrum (EI: 70 eV) 10 most intense m/z: 102, 44, 76, 202, 74, 50, 51, 103, 230, 129. IR (KBr, cm^{-1}): 3062 m, 2976 m, 2890 m, 2212 s, 1599 s, 1480 s, 1378 s, 1228 m, 1029 m, 942 m, 781 s, 684 m, 598 m.

$[Mg_3(O_2CNMe_2)_6(THF)_2]$ (5). ^{1}H NMR [$(CD_3)_2SO$]: δ 1.74 (m, 8H, 3, 4 –thf –*H*), 2.75 [br, 36H, $N(CH_3)_2$], 3.58 (m, 8H, 2, 5 –thf –*H*). ^{13}C NMR [$(CD_3)_2SO$]: δ 25.15 (3, 4 –thf –*C*), 35.93 [$N(CH_3)_2$], 67.02 (2, 5 –thf –*C*), 162.51 (CO_2). Mass spectrum (EI: 70 eV) 10 most intense m/z: 552, 554, 553, 232, 233, 169, 168, 352, 73, 72. IR (KBr, cm^{-1}): 2924 s, 2787 m, 1620 s, 1383 s, 1266 s, 1146 w, 853 s, 812 s, 637 s.

$[Mg_3(O_2CNMe_2)_6(HMPA)_2]$ (6). ^{1}H NMR (C_6D_6): δ 2.42 [br, 36H, $(Me_2N)_3PO$], 2.95 [d, 36H, $N(CH_3)_2$], ^{13}C NMR (C_6D_6): δ 36.73 [$(Me_2N)_3PO$], 36.90 [$(Me_2N)_3PO$], 37.14 [$N(CH_3)_2$], 37.19 [$N(CH_3)_2$], 37.76 [$N(CH_3)_2$], 164.37 (CO_2). ^{31}P NMR (C_6D_6): δ

553, 135, 234, 233, 555, 44, 557. IR (KBr, cm^{-1}): 2995 m, 2883 sh, 2810 s, 2421 w, 1601 s, 1494 s, 1450 s, 1372 s, 1281 s, 1203 s, 1074 m, 1044 s, 985 s, 852 w, 808 s, 750 s, 613 s, 477 s, 447 s.

$[Mg_6(O_2CNEt_2)_{12}]$ (7). ^1H NMR (C_6D_6): δ 1.14 (m, 60H, CH_3), 1.38 (t, 12H, CH_3), 2.89 (m, 16H, CH_2), 3.21 (m, 8H, CH_2), 3.31 (m, 4H, CH_2), 3.43 (m, 4H, CH_2), 3.54 (m, 8H, CH_2), 3.89 (m, 4H, CH_2), 4.35 (m, 4H, CH_2). ^{13}C NMR (C_6D_6): δ 13.46 [$N(CH_2CH_3)_2$], 14.91 [$N(CH_2CH_3)_2$], 14.98 [$N(CH_2CH_3)_2$], 15.07 $N(CH_2CH_3)_2$], 15.78 [$N(CH_2CH_3)_2$], 41.61 [$N(CH_2CH_3)_2$], 41.80 [$N(CH_2CH_3)_2$], 42.90 [$N(CH_2CH_3)_2$], 43.69 [$N(CH_2CH_3)_2$], 43.81 [$N(CH_2CH_3)_2$], 163.26 (CO_2), 163.37 (CO_2), 163.68 (CO_2), 163.97 (CO_2). Mass spectrum (EI: 30 eV) 10 most intense m/z: 692, 695, 44, 58, 42, 697, 696, 290, 288,249. IR (KBr, cm^{-1}): 2962 m, 2932 m, 1622 s, 1554 s, 1527 s, 1491 s, 1428 s, 1319 s, 1100 m, 806 m, 624 m, 460 br.

$[Mg_6(O_2CNPh_2)_{12}]$ (8). ^1H NMR (C_6D_6): δ 6.83~7.63 (m, 120H, C_6H_5). ^1H NMR (C_4D_8O): δ 6.91~7.25 (m, 120H, C_6H_5). ^{13}C NMR (C_4D_8O): δ 117.86 (*p-C*), 117.92 (*p-C*), 120.58 (*m-C*), 126.00 (*m-C*), 128.79 (*o-C*), 129.64 (*o-C*), 144.69 (CO_2), 144.78 (CO_2), 146.57 (CO_2). Mass spectrum (EI: 70 eV) 10 most intense m/e: 169, 168, 167, 91, 92, 84, 51, 77, 65, 115. IR (KBr, cm^{-1}): 3060 m, 3034 m, 2972 m, 2929 m, 2869 w, 2336 w, 1946 w, 1862 w, 1661 s, 1595 s, 1492 s, 1455 s, 1384 br, 1326 s, 1239 s, 1172 m, 1149 m, 1108 w, 1067 m, 1021 m, 945 m, 895 w, 817 s, 794 s 749 s, 694 s, 660 s, 615 m, 505 m.

$[Mg_2(O_2CNPh_2)_4(HMPA)_2]$ 9. ^1H NMR (C_6D_6): δ 2.35 [d, 36H, $N(CH_3)_2$]), 6.83 (t, 8H, *p-H*), 7.03~7.16 (m, 32H, *o/m-H*), ^{13}C NMR (C_6D_6): δ 37.06 [$(Me_2N)_3PO$], 118.43 (*p-C*), 121.05 (*m-C*), 129.79 (*o-C*), 144.39 (CO_2). ^{31}P NMR (C_6D_6): δ 24.75 [$(Me_2N)_3PO$]. Mass spectrum (EI: 70 eV) 10 most intense m/z: 169, 168, 135, 44, 167, 179, 180, 45, 136, 92. IR (KBr, cm^{-1}): 3044 m, 2925 sh, 2850 w, 2807 w, 1596 s, 1495 s, 1455 m, 1368 m, 1314 s, 1248 w, 1196 m, 1069 m, 988 s, 880 w, 851 w, 797 w, 747 s, 697 m, 664 w, 567 w, 509 w, 480 w.

$[Mg_6(\mu_4\text{-}O)(O_2CN^iPr_2)_{10}]\cdot 3THF$, [(10)•3THF]. ^1H NMR (C_6D_6): δ 0.85~1.53 (m, 132 H, $CH(CH_3)_2$ and 3, 4 –thf –*H*), 3.26 [m, 6 H, $CH(CH_3)_2$], 3.61 (t, 12H, 2, 5 –thf –*H*), 3.98 [br, 8H, $CH(CH_3)_2$], 4.45 [br, 2H, $CH(CH_3)_2$], 4.83 [br, 4H, $CH(CH_3)_2$], ^{13}C NMR (C_6D_6): δ 21.21 [$CH(CH_3)_2$], 21.37 [$CH(CH_3)_2$], 21.79 [$CH(CH_3)_2$], 21.92 [$CH(CH_3)_2$], 22.01 [$CH(CH_3)_2$], 22.18 [$CH(CH_3)_2$], 22.32 [$CH(CH_3)_2$], 22.42 [$CH(CH_3)_2$], 23.50 [$CH(CH_3)_2$], 24.09 [$CH(CH_3)_2$],], 26.10 (3, 4 –thf –*C*), 44.14 [$CH(CH_3)_2$], 44.29 [$CH(CH_3)_2$], 44.50 [$CH(CH_3)_2$], 44.67 [$CH(CH_3)_2$], 45.15 [$CH(CH_3)_2$], 45.74 [$CH(CH_3)_2$], 45.97 [$CH(CH_3)_2$], 46.36 [$CH(CH_3)_2$], 46.59 [$CH(CH_3)_2$], 46.95 [$CH(CH_3)_2$], 68.55 (2, 5 –thf –*C*), 161.32 (CO_2), 162.47 (CO_2), 162.72 (CO_2), 162.92 (CO_2), 163.08 (CO_2),163.24 (CO_2), 165.36 (CO_2), 165.50 (CO_2), 165.63 (CO_2), 165.81 (CO_2). Mass spectrum (EI: 70 eV) 10 most intense m/z: 832, 833, 834, 836, 837, 689, 838, 691, 521, 705. IR (KBr, cm^{-1}): 2962 s, 2933 s, 2872 m, 1578 s, 1459 s, 1381 s, 1349 s, 1262 s, 1221 m, 1164 m, 1135 m, 1065 m, 1036 m, 902 w, 868 m, 852 m, 806 m, 782

w, 641 m, 609 m, 527 w.

$[Mg_5(\mu_5, \eta^6\text{-}CO_3)(O_2CN^iPr_2)_8(HMPA)_2]$ (11). ^{1}H NMR (C_6D_6): δ 1.33 [d, 48H, $CH(CH_3)_2$], 2.55 [d, 36H, $(Me_2N)_3PO$], 4.07 [br, 16H, $CH(CH_3)_2$], ^{13}C NMR (C_6D_6): δ 21.09 [$CH(CH_3)_2$], 24.06 [$CH(CH_3)_2$], 37.17 [$(Me_2N)_3PO$], 37.21 [$(Me_2N)_3PO$], 162.49 (CO_2), 163.85 (CO_3). ^{31}P NMR (C_6D_6): δ 23.61 [$(Me_2N)_3PO$]. Mass spectrum (EI: 70 eV) 10 most intense m/z: 833, 835, 837, 834, 345, 344, 388, 386, 58, 86. IR (neat): 2963 s, 2810 w, 2722 w, 1590 s, 1477 sh, 1354 s, 1300 m, 1210 s, 1162 m, 1068 m, 987 s, 856 w, 809 m, 749 m, 613 sh, 528 m, 483 m.

Spectra data:

$[BrMg(\mu\text{-}O_2CPh)(THF)_2]_2$ (1). ^{1}H NMR [$(CD_3)_2SO$]: δ 1.73 (m, 8H, 3, 4 –thf –*H*), 3.57 (m, 8H, 2, 5 –thf –*H*), 7.38~7.41 (m, 3H, *m*-*H*/*p*-*H*), 8.05 (m, 2H, *o*-*H*). ^{13}C NMR [$(CD_3)_2SO$]: δ 25.18 (3, 4 –thf –*C*), 67.08 (2, 5 –thf –*C*), 127.76 (*m*-*C*), 129.82 (*o*-*C*), 131.03 (*p*-*C*), 135.67 (*ipso*-*C*), 172.25 (CO_2). Mass spectrum (EI: 70 eV) 10 most intense m/z: 42, 44, 78, 71, 72, 77, 69, 79, 105, 122. IR (KBr, cm^{-1}): 3069 s, 2889 s, 1626 br, 1573 s, 1494 s, 1428 s, 1314 s, 1176 s, 1035 s, 920 s, 880 s, 719 s, 673 s.

$[Mg_3(O_2C^iPr)_6(THF)_2]$ (2). ^{1}H NMR [$(CD_3)_2SO$]: δ 0.98 [d, 36H, $CH(CH_3)_2$], 1.76 (m, 8H, 3, 4 –thf –*H*), 2.26 [m, 6H, $CH(CH_3)_2$], 3.60 (m, 8H, 2, 5 –thf –*H*). ^{13}C NMR [$(CD_3)_2SO$]: δ 19.81 [$CH(CH_3)_2$], 25.12 (3, 4 –thf –*C*), 34.90 [$CH(CH_3)_2$], 67.02 (2, 5 –thf –*C*), 183.84 (CO_2). Mass spectrum (EI: 70 eV) 10 most intense m/z: 547, 549, 548, 230, 43, 231, 41, 550, 44, 551. IR (KBr, cm^{-1}): 2923 s, 2853 sh, 1582 m, 1457 s, 1372 m, 1295 w, 1169 w, 1100 w, 1073 w, 1038 w, 928 m, 891 w, 853 w, 787 w, 722 w, 673 w, 561 w.

$[Mg_3(O_2C^iPr)_6(HMPA)_2]$ (3). ^{1}H NMR (C_6D_6): δ 1.39 [d, 36H, $CH(CH_3)_2$], 2.39 [d, 36H, $(Me_2N)_3PO$], 2.84 [br, 6H, $CH(CH_3)_2$], ^{13}C NMR (C_6D_6): δ 20.72 [$CH(CH_3)_2$], 37.06 [$CH(CH_3)_2$], 37.11 [$(Me_2N)_3PO$], 185.42 (CO_2). ^{31}P NMR (C_6D_6): δ 24.09 [$(Me_2N)_3PO$]. Mass spectrum (EI: 70 eV) 10 most intense m/z: 135, 44, 179, 46, 180, 92, 136, 47, 93, 90. IR (KBr, cm^{-1}): 2966 s, 2923 sh, 2811 m, 1604 s, 1555 s, 1465 s, 1416 s, 1373 m, 1356 m, 1304 s, 1208 s, 1131 m, 1093 m, 1070 m, 991 s, 944 w, 928 w, 861 w, 837 w, 609 m, 531 w, 477 s, 420 s.

$[Mg_3(O_2CC{\equiv}CPh)_6(THF)_2]$ (4). ^{1}H NMR [$(CD_3)_2SO$]: δ 1.74 (m, 8H, 3, 4 –thf –*H*), 3.59 (m, 8H, 2, 5 –thf –*H*), 7.36~7.46 (m, 30H, C_6H_5), ^{13}C NMR [$(CD_3)_2SO$]: δ 25.15 (3, 4 –thf –*C*), 67.04 (2, 5 –thf –*C*), 76.21 (*C*≡CPh), 89.46 (C≡*C*Ph), 122.13 (*ipso*-*C*), 128.72 (*p*-*C*), 128.78 (*m*-*C*), 131.66 (*o*-*C*), 156.54 (CO_2). Mass spectrum (EI: 70 eV) 10 most intense m/z: 102, 44, 76, 202, 74, 50, 51, 103, 230, 129. IR (KBr, cm^{-1}): 3062 m, 2976 m, 2890 m, 2212 s, 1599 s, 1480 s, 1378 s, 1228 m, 1029 m, 942 m, 781 s, 684 m, 598 m.

$[Mg_3(O_2CNMe_2)_6(THF)_2]$ (5). ^{1}H NMR [$(CD_3)_2SO$]: δ 1.74 (m, 8H, 3, 4 –thf –*H*), 2.75 [br, 36H, $N(CH_3)_2$], 3.58 (m, 8H, 2, 5 –thf –*H*). ^{13}C NMR [$(CD_3)_2SO$]: δ 25.15 (3, 4 –thf –*C*), 35.93 [$N(CH_3)_2$], 67.02 (2, 5 –thf –*C*), 162.51 (CO_2). Mass spectrum (EI: 70 eV) 10 most intense m/z: 552, 554, 553, 232, 233, 169, 168, 352, 73, 72. IR (KBr, cm^{-1}): 2923 s, 2853 sh, 1582 m, 1457 s, 1372 m, 1295 w, 1169 w, 1100 w, 1073 w, 1038 w, 928 m, 891 w, 853 w, 787 w, 722 w, 673 w.

$[Mg_3(O_2CNMe_2)_6(HMPA)_2]$ (6). ^{1}H NMR (C_6D_6): δ 2.42 [br, 36H, $(Me_2N)_3PO$], 2.95 [d, 36H, $N(CH_3)_2$], ^{13}C NMR (C_6D_6): δ 36.73 [$(Me_2N)_3PO$], 36.90 [$(Me_2N)_3PO$], 37.14 [$N(CH_3)_2$], 37.19 [$N(CH_3)_2$], 37.76 [$N(CH_3)_2$], 164.37 (CO_2). ^{31}P NMR (C_6D_6): δ 24.13 [$(Me_2N)_3PO$]. Mass spectrum (EI: 70 eV) 10 most intense m/z: 552, 232, 554,

553, 135, 234, 233, 555, 44, 557. IR (KBr, cm^{-1}): 2995 m, 2883 sh, 2810 s, 2421 w, 1601 s, 1494 s, 1450 s, 1372 s, 1281 s, 1203 s, 1074 m, 1044 s, 985 s, 852 w, 808 s, 750 s, 613 s, 477 s, 447 s.

$[Mg_6(O_2CNEt_2)_{12}]$ (7). ^1H NMR (C_6D_6): δ 1.14 (m, 60H, CH_3), 1.38 (t, 12H, CH_3), 2.89 (m, 16H, CH_2), 3.21 (m, 8H, CH_2), 3.31 (m, 4H, CH_2), 3.43 (m, 4H, CH_2), 3.54 (m, 8H, CH_2), 3.89 (m, 4H, CH_2), 4.35 (m, 4H, CH_2). ^{13}C NMR (C_6D_6): δ 13.46 [$N(CH_2CH_3)_2$], 14.91 [$N(CH_2CH_3)_2$], 14.98 [$N(CH_2CH_3)_2$], 15.07 $N(CH_2CH_3)_2$], 15.78 [$N(CH_2CH_3)_2$], 41.61 [$N(CH_2CH_3)_2$], 41.80 [$N(CH_2CH_3)_2$], 42.90 [$N(CH_2CH_3)_2$], 43.69 [$N(CH_2CH_3)_2$], 43.81 [$N(CH_2CH_3)_2$], 163.26 (CO_2), 163.37 (CO_2), 163.68 (CO_2), 163.97 (CO_2). Mass spectrum (EI: 30 eV) 10 most intense m/z: 692, 695, 44, 58, 42, 697, 696, 290, 288,249. IR (KBr, cm^{-1}): 2962 m, 2932 m, 1622 s, 1554 s, 1527 s, 1491 s, 1428 s, 1319 s, 1100 m, 806 m, 624 m, 460 br.

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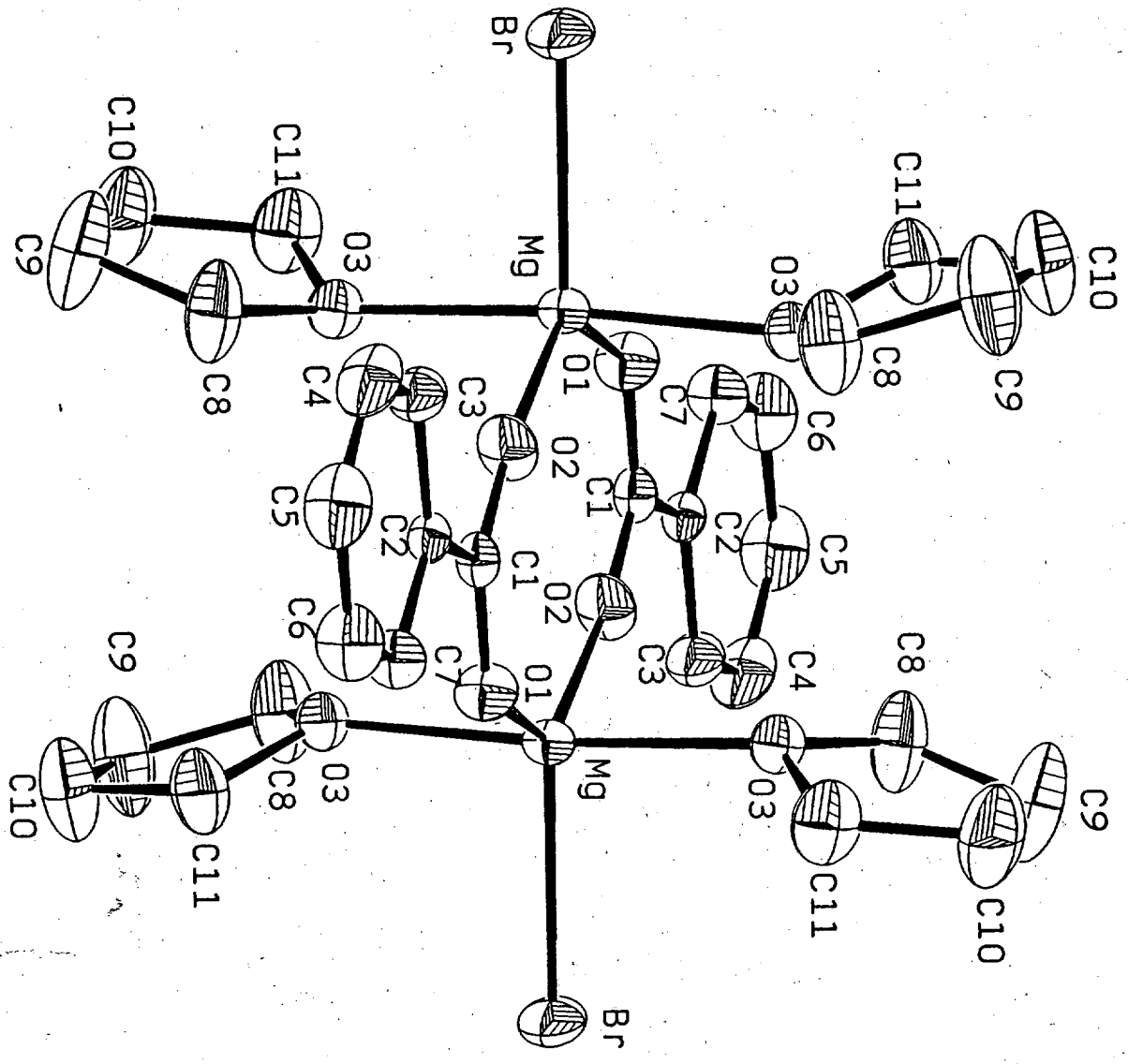
$[Mg_6(\mu_4\text{-}O)(O_2CN^iPr_2)_{10}]\cdot 3THF$, [(10)•3THF]. ^1H NMR (C_6D_6): δ 0.85~1.53 (m, 132 H, $CH(CH_3)_2$ and 3, 4 –thf –*H*), 3.26 [m, 6 H, $CH(CH_3)_2$], 3.61 (t, 12H, 2, 5 –thf –*H*), 3.98 [br, 8H, $CH(CH_3)_2$], 4.45 [br, 2H, $CH(CH_3)_2$], 4.83 [br, 4H, $CH(CH_3)_2$], ^{13}C NMR (C_6D_6): δ 21.21 [$CH(CH_3)_2$], 21.37 [$CH(CH_3)_2$], 21.79 [$CH(CH_3)_2$], 21.92 [$CH(CH_3)_2$], 22.01 [$CH(CH_3)_2$], 22.18 [$CH(CH_3)_2$], 22.32 [$CH(CH_3)_2$], 22.42 [$CH(CH_3)_2$], 23.50 [$CH(CH_3)_2$], 24.09 [$CH(CH_3)_2$],], 26.10 (3, 4 –thf –*C*), 44.14 [$CH(CH_3)_2$], 44.29 [$CH(CH_3)_2$], 44.50 [$CH(CH_3)_2$], 44.67 [$CH(CH_3)_2$], 45.15 [$CH(CH_3)_2$], 45.74 [$CH(CH_3)_2$], 45.97 [$CH(CH_3)_2$], 46.36 [$CH(CH_3)_2$], 46.59 [$CH(CH_3)_2$], 46.95 [$CH(CH_3)_2$], 68.55 (2, 5 –thf –*C*), 161.32 (CO_2), 162.47 (CO_2), 162.72 (CO_2), 162.92 (CO_2), 163.08 (CO_2),163.24 (CO_2), 165.36 (CO_2), 165.50 (CO_2), 165.63 (CO_2), 165.81 (CO_2). Mass spectrum (EI: 70 eV) 10 most intense m/z: 832, 833, 834, 836, 837, 689, 838, 691, 521, 705. IR (KBr, cm^{-1}): 2962 s, 2933 s, 2872 m, 1578 s, 1459 s, 1381 s, 1349 s, 1262 s, 1221 m, 1164 m, 1135 m, 1065 m, 1036 m, 902 w, 868 m, 852 m, 806 m, 782

w, 641 m, 609 m, 527 w.

$[Mg_5(\mu_5, \eta^6\text{-}CO_3)(O_2CN^iPr_2)_8(HMPA)_2]$ (11). ^{1}H NMR (C_6D_6): δ 1.33 [d, 48H, $CH(CH_3)_2$], 2.55 [d, 36H, $(Me_2N)_3PO$], 4.07 [br, 16H, $CH(CH_3)_2$], ^{13}C NMR (C_6D_6): δ 21.09 [$CH(CH_3)_2$], 24.06 [$CH(CH_3)_2$], 37.17 [$(Me_2N)_3PO$], 37.21 [$(Me_2N)_3PO$], 162.49 (CO_2), 163.85 (CO_3). ^{31}P NMR (C_6D_6): δ 23.61 [$(Me_2N)_3PO$]. Mass spectrum (EI: 70 eV) 10 most intense m/z: 833, 835, 837, 834, 345, 344, 388, 386, 58, 86. IR (neat): 2963 s, 2810 w, 2722 w, 1590 s, 1477 sh, 1354 s, 1300 m, 1210 s, 1162 m, 1068 m, 987 s, 856 w, 809 m, 749 m, 613 sh, 528 m, 483 m.



IC48

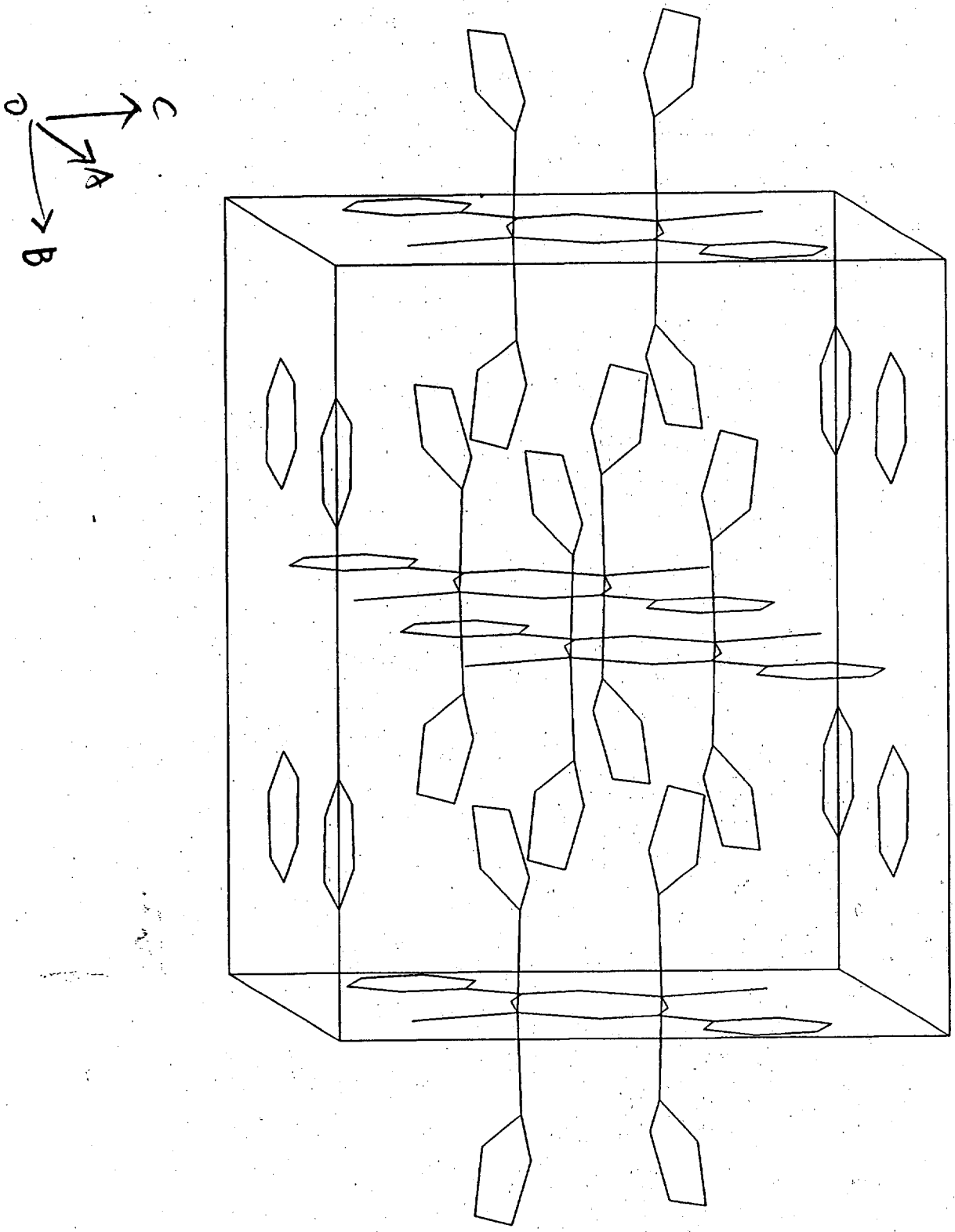

c
a
b

Table. Crystal Data and Conditions for Crystallographic Data Collection and Structure Refinement

TITLE	*** IC4827 ***
Formula	C36 H48 O8 Mg2 Br2
Formular wt	817.19
Diffractometer used	Nonius
Space Group	Monoclinic C 2/m
a (angstron)	11.436(5)
b (angstron)	15.918(5)
c (angstron)	12.271(3)
beta (deg.)	99.79(3)
V (A**3)	2201.3(13)
Z	2
Dcalc. (g.cm**-3)	1.233
lambda (Angstron)	0.7107
F(000)	844.
Unit cell detn: #;(2theta range)	25;(17.76 - 31.00 deg.)
Scan type	theta/2theta
Scan width (deg.)	2(0.70+0.35tan(theta))
Scan Speed (deg./min)	2.75-8.24
(2Theta)max.	50.0
h k l ranges	(-13; 13)(0; 18)(0; 14)
mu (cm**-1)	18.895
Crystal size (mm)	0.80 X 1.00 X 1.00
Transmission	0.735; 1.000
Temperature (K)	298.
# of meas. reflns.	2055
# of obsed relfns. (I>2.0sig(I))	1313
# of unique reflns.	2040
Rf;Rw	0.039;0.038
GoF	2.14
Refinement program	NRCVAX
# of atoms	37
# of refined params.	141 (1313 out of 2040 reflns.)
Minimize function	Sum(w|Fo-Fc|**2)
Unit weights were used	
g (2nd. ext. coeff.) x 10E4	1.25(3)
(delta/sigma)max.	0.0020
Residual in final D-map (e/A**3)	-0.400; 0.420

NOTE :

Rf = Sum(Fo-Fc)/Sum(Fo)

Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)]

GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]

3 standard reflections (6,0,0 ; 0,12,0 ; 1,1,7) monitored every 3600 seconds, intensity decay 7%.

Solvent : C6H6

Table : Bond Distances and Bond Angles of IC4827

Mg-Br	2.4997(20)	C3-C4	1.439(10)
Mg-O1	1.983(4)	C4-C5	1.347(13)
Mg-O2	1.930(4)	C5-C6	1.318(12)
Mg-O3	2.104(3)	C6-C7	1.380(8)
Mg-O3	2.104(3)	C8-C9	1.465(8)
O1-C1	1.255(7)	C9-C10	1.430(10)
O2-C1	1.233(7)	C10-C11	1.458(9)
O3-C8	1.422(6)	C12-C13	1.367(9)
O3-C11	1.425(6)	C12-C13	1.367(9)
C1-O2	1.233(7)	C13-C14	1.343(11)
C1-C2	1.490(7)	C14-C15	1.336(8)
C2-C3	1.374(7)	C15-C14	1.336(8)
C2-C7	1.370(8)		

Br-Mg-O1	114.45(14)	O2-C1-C2	118.6(5)
Br-Mg-O2	118.02(17)	C1-C2-C3	120.9(5)
Br-Mg-O3	92.28(9)	C1-C2-C7	120.2(5)
Br-Mg-O3	92.28(9)	C3-C2-C7	118.9(5)
O1-Mg-O2	127.52(21)	C2-C3-C4	118.2(6)
O1-Mg-O3	89.76(9)	C3-C4-C5	119.6(6)
O1-Mg-O3	89.76(9)	C4-C5-C6	121.8(7)
O2-Mg-O3	88.24(9)	C5-C6-C7	119.9(7)
O2-Mg-O3	88.24(9)	C2-C7-C6	121.6(6)
O3-Mg-O3	175.18(14)	O3-C8-C9	107.7(5)
Mg-O1-C1	123.1(4)	C8-C9-C10	106.9(5)
Mg-O2-C1	165.5(4)	C9-C10-C11	107.6(5)
Mg-O3-C8	121.8(3)	O3-C11-C10	106.8(5)
Mg-O3-C11	122.0(3)	C13-C12-C13	119.6(7)
C8-O3-C11	108.6(4)	C12-C13-C14	119.2(6)
O1-C1-O2	123.9(5)	C13-C14-C15	120.9(6)
O1-C1-C2	117.6(5)	C14-C15-C14	120.2(8)

Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

	u11(U)	u22	u33	u12	u13	u23
Mg	3.77(9)	5.72(12)	3.86(9)	0.0	0.94(7)	0.0
Br	12.14(6)	8.74(5)	4.36(3)	0.0	-1.05(3)	0.0
O1	6.7 (3)	8.3 (3)	5.11(22)	0.0	2.59(20)	0.0
O2	3.54(22)	7.2 (3)	11.5 (4)	0.0	1.31(23)	0.0
O3	6.09(17)	5.65(18)	6.68(17)	0.36(15)	1.72(14)	-0.06(15)
C1	4.5 (3)	3.6 (3)	5.9 (3)	0.0	1.7 (3)	0.0
C2	4.9 (3)	3.7 (3)	4.0 (3)	0.0	1.40(25)	0.0
C3	9.6 (5)	6.5 (4)	4.8 (3)	0.0	0.4 (3)	0.0
C4	17.9 (9)	7.8 (5)	3.9 (3)	0.0	3.7 (4)	0.0
C5	11.5 (6)	9.2 (6)	10.0 (6)	0.0	6.3 (5)	0.0
C6	7.0 (5)	9.4 (6)	10.7 (6)	0.0	4.8 (4)	0.0
C7	4.5 (4)	7.7 (4)	6.4 (4)	0.0	2.4 (3)	0.0
C8	12.0 (5)	6.8 (4)	18.6 (7)	-0.1 (4)	8.7 (5)	2.0 (4)
C9	18.4 (7)	6.9 (4)	22.9 (8)	2.5 (5)	11.8 (7)	4.6 (5)
C10	14.8 (6)	6.9 (4)	20.9 (8)	2.7 (4)	5.4 (6)	1.8 (5)
C11	9.5 (4)	8.1 (4)	13.7 (5)	2.6 (3)	4.4 (4)	-0.1 (4)
C12	21.8 (11)	7.9 (6)	11.3 (7)	0.0	9.0 (7)	0.0
C13	13.1 (5)	14.3 (6)	10.7 (5)	4.5 (5)	2.9 (4)	2.1 (4)
C14	10.2 (4)	14.5 (6)	10.9 (5)	-2.1 (4)	1.5 (4)	-1.3 (4)
C15	16.6 (9)	8.4 (6)	10.3 (6)	0.0	4.1 (6)	0.0
H3	8.3					
H4	10.8					
H5	10.8					
H6	10.1					
H7	7.3					
H8a	13.5					
H8b	13.5					
H9a	16.0					
H9b	16.0					
H10a	14.8					
H10b	14.8					
H11a	11.5					
H11b	11.5					
H12	14.0					
H13	13.8					
H14	13.0					
H15	12.4					

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+---+2*h*k*u12*astar*bstar+---)

Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

	u11(U)	u22	u33	u12	u13	u23
Mg	3.77(9)	5.72(12)	3.86(9)	0.0	0.94(7)	0.0
Br	12.14(6)	8.74(5)	4.36(3)	0.0	-1.05(3)	0.0
O1	6.7 (3)	8.3 (3)	5.11(22)	0.0	2.59(20)	0.0
O2	3.54(22)	7.2 (3)	11.5 (4)	0.0	1.31(23)	0.0
O3	6.09(17)	5.65(18)	6.68(17)	0.36(15)	1.72(14)	-0.06(15)
C1	4.5 (3)	3.6 (3)	5.9 (3)	0.0	1.7 (3)	0.0
C2	4.9 (3)	3.7 (3)	4.0 (3)	0.0	1.40(25)	0.0
C3	9.6 (5)	6.5 (4)	4.8 (3)	0.0	0.4 (3)	0.0
C4	17.9 (9)	7.8 (5)	3.9 (3)	0.0	3.7 (4)	0.0
C5	11.5 (6)	9.2 (6)	10.0 (6)	0.0	6.3 (5)	0.0
C6	7.0 (5)	9.4 (6)	10.7 (6)	0.0	4.8 (4)	0.0
C7	4.5 (4)	7.7 (4)	6.4 (4)	0.0	2.4 (3)	0.0
C8	12.0 (5)	6.8 (4)	18.6 (7)	-0.1 (4)	8.7 (5)	2.0 (4)
C9	18.4 (7)	6.9 (4)	22.9 (8)	2.5 (5)	11.8 (7)	4.6 (5)
C10	14.8 (6)	6.9 (4)	20.9 (8)	2.7 (4)	5.4 (6)	1.8 (5)
C11	9.5 (4)	8.1 (4)	13.7 (5)	2.6 (3)	4.4 (4)	-0.1 (4)
C12	21.8 (11)	7.9 (6)	11.3 (7)	0.0	9.0 (7)	0.0
C13	13.1 (5)	14.3 (6)	10.7 (5)	4.5 (5)	2.9 (4)	2.1 (4)
C14	10.2 (4)	14.5 (6)	10.9 (5)	-2.1 (4)	1.5 (4)	-1.3 (4)
C15	16.6 (9)	8.4 (6)	10.3 (6)	0.0	4.1 (6)	0.0
H3	8.3					
H4	10.8					
H5	10.8					
H6	10.1					
H7	7.3					
H8a	13.5					
H8b	13.5					
H9a	16.0					
H9b	16.0					
H10a	14.8					
H10b	14.8					
H11a	11.5					
H11b	11.5					
H12	14.0					
H13	13.8					
H14	13.0					
H15	12.4					

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+---+2*h*k*u12*astar*bstar+---)

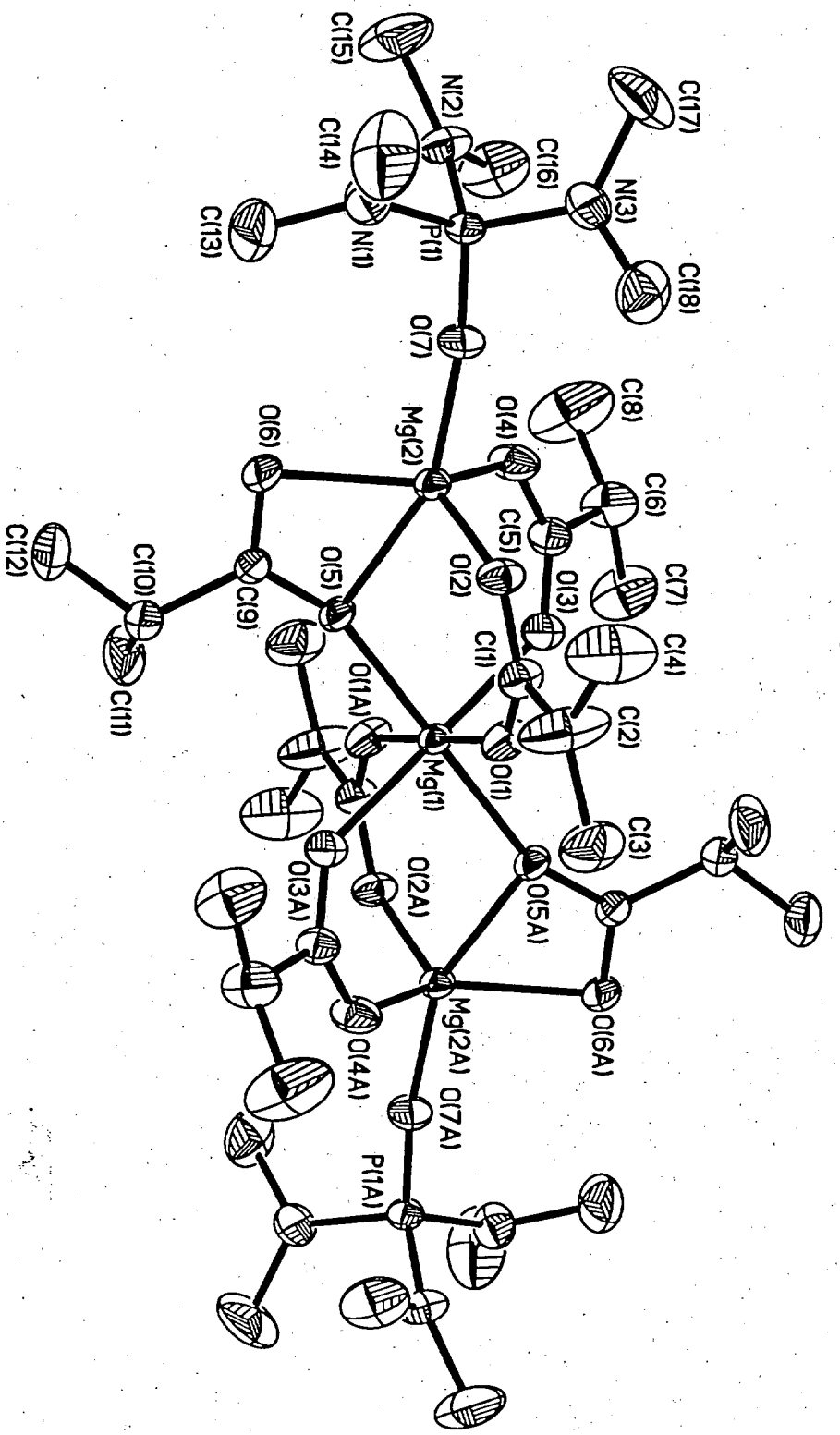


Fig. 1: The molecular structure of IC6329, thermal ellipsoids drawn at the 30% probability level.

Table 1. Crystal data and structure refinement for 6329.

Identification code	ic6329
Empirical formula	$C_{36}H_{78}Mg_3N_6O_{14}P_2$
Formula weight	953.91
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 24.5444(5) Å alpha = 90° b = 11.51080(10) Å beta = 91.1010(10)° c = 18.7256(4) Å gamma = 90°
Volume, Z	5289.5(2) Å^3, 4
Density (calculated)	1.198 Mg/m^3
Absorption coefficient	0.178 mm^{-1}
F(000)	2056
Crystal size	0.70 x 0.40 x 0.40 mm
θ range for data collection	1.66 to 26.38°
Limiting indices	$-30 \le h \le 30$, $-14 \le k \le 8$, $-23 \le l \le 23$
Reflections collected	12524
Independent reflections	5379 (R_{int} = 0.0331)
Absorption correction	empirical used sadabs
Max. and min. transmission	0.9280 and 0.7230
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5379 / 0 / 277
Goodness-of-fit on F^2	1.019
Final R indices [I>2σ(I)]	R1 = 0.0594, wR2 = 0.1536
R indices (all data)	R1 = 0.0900, wR2 = 0.1708
Largest diff. peak and hole	0.596 and -0.365 eÅ^{-3}

Table 2. Bond lengths [Å] and angles [°] for 6329.

Mg(1)-O(1)#1	2.052(2)	Mg(1)-O(1)	2.052(2)
Mg(1)-O(3)#1	2.068(2)	Mg(1)-O(3)	2.068(2)
Mg(1)-O(5)#1	2.075(2)	Mg(1)-O(5)	2.075(2)
Mg(1)-Mg(2)#1	3.4961(8)	Mg(1)-Mg(2)	3.4962(8)
Mg(2)-O(7)	1.948(2)	Mg(2)-O(2)	1.964(2)
Mg(2)-O(4)	1.968(2)	Mg(2)-O(6)	2.091(2)
Mg(2)-O(5)	2.181(2)	P(1)-O(7)	1.476(2)
P(1)-N(2)	1.626(3)	P(1)-N(3)	1.632(3)
P(1)-N(1)	1.632(3)	O(1)-C(1)	1.236(3)
O(2)-C(1)	1.263(3)	O(3)-C(5)	1.241(3)
O(4)-C(5)	1.264(3)	O(5)-C(9)	1.266(3)
O(6)-C(9)	1.257(3)	N(1)-C(14)	1.431(5)
N(1)-C(13)	1.458(5)	N(2)-C(15)	1.462(5)
N(2)-C(16)	1.467(5)	N(3)-C(17)	1.459(5)
N(3)-C(18)	1.469(5)	C(1)-C(2)	1.512(4)
C(2)-C(4)	1.422(6)	C(2)-C(3)	1.440(5)
C(5)-C(6)	1.528(4)	C(6)-C(8)	1.439(6)
C(6)-C(7)	1.499(5)	C(9)-C(10)	1.514(4)
C(10)-C(11)	1.503(5)	C(10)-C(12)	1.510(5)

O(1)#1-Mg(1)-O(1)	180.0	O(1)#1-Mg(1)-O(3)#1	92.07(9)
O(1)-Mg(1)-O(3)#1	87.92(9)	O(1)#1-Mg(1)-O(3)	87.93(9)
O(1)-Mg(1)-O(3)	92.07(9)	O(3)#1-Mg(1)-O(3)	180.0
O(1)#1-Mg(1)-O(5)#1	89.24(7)	O(1)-Mg(1)-O(5)#1	90.76(7)
O(3)#1-Mg(1)-O(5)#1	88.42(8)	O(3)-Mg(1)-O(5)#1	91.58(8)
O(1)#1-Mg(1)-O(5)	90.76(7)	O(1)-Mg(1)-O(5)	89.24(7)
O(3)#1-Mg(1)-O(5)	91.58(8)	O(3)-Mg(1)-O(5)	88.42(8)
O(5)#1-Mg(1)-O(5)	180.0	O(1)#1-Mg(1)-Mg(2)#1	67.73(6)
O(1)-Mg(1)-Mg(2)#1	112.27(6)	O(3)#1-Mg(1)-Mg(2)#1	62.45(6)
O(3)-Mg(1)-Mg(2)#1	117.55(6)	O(5)#1-Mg(1)-Mg(2)#1	35.77(5)
O(5)-Mg(1)-Mg(2)#1	144.23(5)	O(1)#1-Mg(1)-Mg(2)	112.27(6)
O(1)-Mg(1)-Mg(2)	67.73(6)	O(3)#1-Mg(1)-Mg(2)	117.55(6)
O(3)-Mg(1)-Mg(2)	62.45(6)	O(5)#1-Mg(1)-Mg(2)	144.23(5)
O(5)-Mg(1)-Mg(2)	35.77(5)	Mg(2)#1-Mg(1)-Mg(2)	180.0
O(7)-Mg(2)-O(2)	98.43(9)	O(7)-Mg(2)-O(4)	96.86(9)
O(2)-Mg(2)-O(4)	117.75(10)	O(7)-Mg(2)-O(6)	96.39(9)
O(2)-Mg(2)-O(6)	114.14(10)	O(4)-Mg(2)-O(6)	123.45(10)
O(7)-Mg(2)-O(5)	157.18(9)	O(2)-Mg(2)-O(5)	94.00(8)
O(4)-Mg(2)-O(5)	94.13(8)	O(6)-Mg(2)-O(5)	60.96(7)
O(7)-Mg(2)-Mg(1)	169.03(7)	O(2)-Mg(2)-Mg(1)	75.45(6)
O(4)-Mg(2)-Mg(1)	78.49(6)	O(6)-Mg(2)-Mg(1)	94.45(6)
O(5)-Mg(2)-Mg(1)	33.79(5)	O(7)-P(1)-N(2)	110.74(13)
O(7)-P(1)-N(3)	109.13(13)	N(2)-P(1)-N(3)	110.1(2)
O(7)-P(1)-N(1)	111.96(14)	N(2)-P(1)-N(1)	106.6(2)
N(3)-P(1)-N(1)	108.3(2)	C(1)-O(1)-Mg(1)	139.4(2)
C(1)-O(2)-Mg(2)	131.1(2)	C(5)-O(3)-Mg(1)	140.6(2)
C(5)-O(4)-Mg(2)	124.5(2)	C(9)-O(5)-Mg(1)	158.1(2)
C(9)-O(5)-Mg(2)	87.9(2)	Mg(1)-O(5)-Mg(2)	110.44(8)
C(9)-O(6)-Mg(2)	92.2(2)	P(1)-O(7)-Mg(2)	171.0(2)
C(14)-N(1)-C(13)	115.1(3)	C(14)-N(1)-P(1)	125.5(3)
C(13)-N(1)-P(1)	119.2(3)	C(15)-N(2)-C(16)	115.4(3)
C(15)-N(2)-P(1)	124.2(3)	C(16)-N(2)-P(1)	119.8(2)
C(17)-N(3)-C(18)	113.8(3)	C(17)-N(3)-P(1)	124.3(3)
C(18)-N(3)-P(1)	120.4(2)	O(1)-C(1)-O(2)	125.9(3)
O(1)-C(1)-C(2)	116.8(3)	O(2)-C(1)-C(2)	117.2(3)
C(4)-C(2)-C(3)	122.9(4)	C(4)-C(2)-C(1)	116.2(4)
C(3)-C(2)-C(1)	117.5(3)	O(3)-C(5)-O(4)	124.2(3)
O(3)-C(5)-C(6)	118.4(3)	O(4)-C(5)-C(6)	117.3(3)
C(8)-C(6)-C(7)	115.1(4)	C(8)-C(6)-C(5)	113.6(3)

C(7)-C(6)-C(5)	112.5(3)	O(6)-C(9)-O(5)	118.5(2)
O(6)-C(9)-C(10)	121.5(2)	O(5)-C(9)-C(10)	120.0(2)
C(11)-C(10)-C(12)	113.6(3)	C(11)-C(10)-C(9)	110.7(3)
C(12)-C(10)-C(9)	112.4(3)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z

Table 3. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 6329. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Mg(1)	5000	5000	0	32(1)
Mg(2)	3634(1)	4917(1)	492(1)	33(1)
P(1)	2279(1)	5149(1)	846(1)	38(1)
O(1)	4785(1)	6421(2)	593(1)	51(1)
O(2)	3922(1)	6344(2)	933(1)	46(1)
O(3)	4417(1)	5370(2)	-779(1)	52(1)
O(4)	3566(1)	4869(2)	-556(1)	52(1)
O(5)	4419(1)	4029(2)	525(1)	40(1)
O(6)	3727(1)	3434(2)	1128(1)	51(1)
O(7)	2864(1)	5161(2)	679(1)	48(1)
N(1)	2174(1)	4737(3)	1666(2)	60(1)
N(2)	1950(1)	4239(3)	332(2)	58(1)
N(3)	2031(1)	6455(2)	742(2)	55(1)
C(1)	4392(1)	6786(2)	931(2)	43(1)
C(2)	4492(2)	7834(4)	1404(3)	107(2)
C(3)	5023(2)	8367(4)	1385(3)	83(1)
C(4)	4021(2)	8430(4)	1639(3)	125(2)
C(5)	3952(1)	5073(3)	-976(2)	44(1)
C(6)	3823(2)	5015(4)	-1777(2)	69(1)
C(7)	4327(2)	4991(4)	-2217(2)	94(2)
C(8)	3419(2)	4157(6)	-1966(2)	139(3)
C(9)	4224(1)	3352(2)	988(2)	40(1)
C(10)	4593(1)	2502(3)	1380(2)	58(1)
C(11)	4902(2)	1768(4)	861(2)	86(1)
C(12)	4295(2)	1804(4)	1932(2)	78(1)
C(13)	2433(2)	3677(4)	1931(2)	91(1)
C(14)	1885(3)	5387(5)	2188(3)	133(2)
C(15)	1458(2)	3617(5)	538(3)	111(2)
C(16)	2090(2)	4147(4)	-424(2)	93(1)
C(17)	1459(2)	6708(5)	583(3)	110(2)
C(18)	2350(2)	7474(3)	969(2)	84(1)

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 5464. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Mg(1)	79(1)	35(1)	67(1)	0	-4(1)	0
Mg(2)	81(1)	44(1)	74(1)	-10(1)	-7(1)	5(1)
O(1)	92(1)	43(1)	88(2)	-12(1)	-17(1)	3(1)
O(2)	90(1)	46(1)	96(2)	-17(1)	-16(1)	6(1)
O(3)	78(1)	39(1)	64(1)	1(1)	-2(1)	2(1)
O(4)	77(1)	55(1)	67(1)	1(1)	-3(1)	7(1)
O(5)	100(2)	54(1)	80(2)	-6(1)	-16(1)	16(1)
O(6)	83(2)	78(2)	118(2)	-11(2)	6(1)	10(1)
N(1)	122(2)	56(2)	145(3)	-39(2)	-54(2)	16(2)
N(2)	108(3)	68(2)	50(2)	0	0	-9(2)
N(3)	124(2)	57(2)	96(2)	6(2)	-32(2)	18(2)
N(4)	72(3)	97(3)	138(4)	-44(3)	0	0
C(1)	99(3)	46(2)	84(2)	-13(2)	-8(2)	-7(2)
C(2)	314(10)	87(4)	183(7)	-56(5)	-104(7)	56(5)
C(3)	163(6)	149(7)	433(16)	-116(10)	-119(9)	46(5)
C(4)	145(4)	65(2)	158(5)	-31(3)	-36(3)	14(3)
C(5)	230(7)	114(5)	255(9)	52(5)	-16(6)	23(5)
C(6)	75(3)	41(2)	67(3)	0	0	8(2)
C(7)	127(3)	92(3)	67(2)	10(2)	5(2)	-5(2)
C(8)	160(4)	105(3)	144(4)	45(3)	-6(3)	5(3)
C(9)	80(2)	48(2)	77(2)	0(2)	-1(2)	11(2)
C(10)	170(5)	90(3)	142(4)	16(3)	-58(4)	27(3)
C(11)	156(5)	177(6)	181(6)	-42(5)	-56(5)	64(5)
C(12)	153(4)	49(2)	152(4)	5(2)	-40(3)	17(3)
C(13)	174(5)	98(4)	196(6)	-44(4)	-44(5)	44(3)
C(14)	78(3)	86(4)	83(4)	-6(3)	0	0
C(15)	92(3)	140(5)	186(6)	-69(4)	-17(3)	1(3)
C(16)	310(12)	174(7)	273(10)	-25(6)	6(8)	-138(8)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 5464.

	x	y	z	U(eq)
H(2B)	3344(5)	30(3)	5536(4)	233
H(2C)	3125(5)	622(3)	5673(4)	233
H(3A)	3265(4)	457(3)	4330(6)	372
H(3B)	3974(4)	293(3)	4502(6)	372
H(3C)	3756(4)	882(3)	4638(6)	372
H(4B)	4931(2)	205(2)	6215(3)	147
H(4C)	4548(2)	-140(2)	5584(3)	147
H(5A)	4612(3)	-572(2)	6819(5)	299
H(5B)	3897(3)	-437(2)	6627(5)	299
H(5C)	4281(3)	-91(2)	7258(5)	299
H(7A)	5500(2)	2754(2)	4406(2)	114
H(7B)	5694(2)	3037(2)	5227(2)	114
H(8A)	5168(3)	3623(2)	4385(3)	205
H(8B)	4765(3)	3530(2)	5183(3)	205
H(8C)	4571(3)	3248(2)	4362(3)	205
H(10A)	3133(3)	3864(2)	4990(3)	161
H(10B)	3381(3)	3281(2)	4903(3)	161
H(11A)	2298(3)	3297(2)	4842(4)	257
H(11B)	2266(3)	3565(2)	5710(4)	257
H(11C)	2514(3)	2981(2)	5623(4)	257
H(12A)	3699(2)	4367(2)	5941(3)	142
H(12B)	3993(2)	4111(2)	6733(3)	142
H(13A)	3149(3)	4656(2)	7089(4)	234
H(13B)	2983(3)	4068(2)	7322(4)	234
H(13C)	2689(3)	4323(2)	6530(4)	234
H(15A)	1210(2)	2239(2)	6773(4)	167
H(15B)	1837(2)	1905(2)	6704(4)	167
H(16A)	1066(4)	1429(3)	7296(5)	378
H(16B)	995(4)	1856(3)	7990(5)	378
H(16C)	1624(4)	1522(3)	7922(5)	378

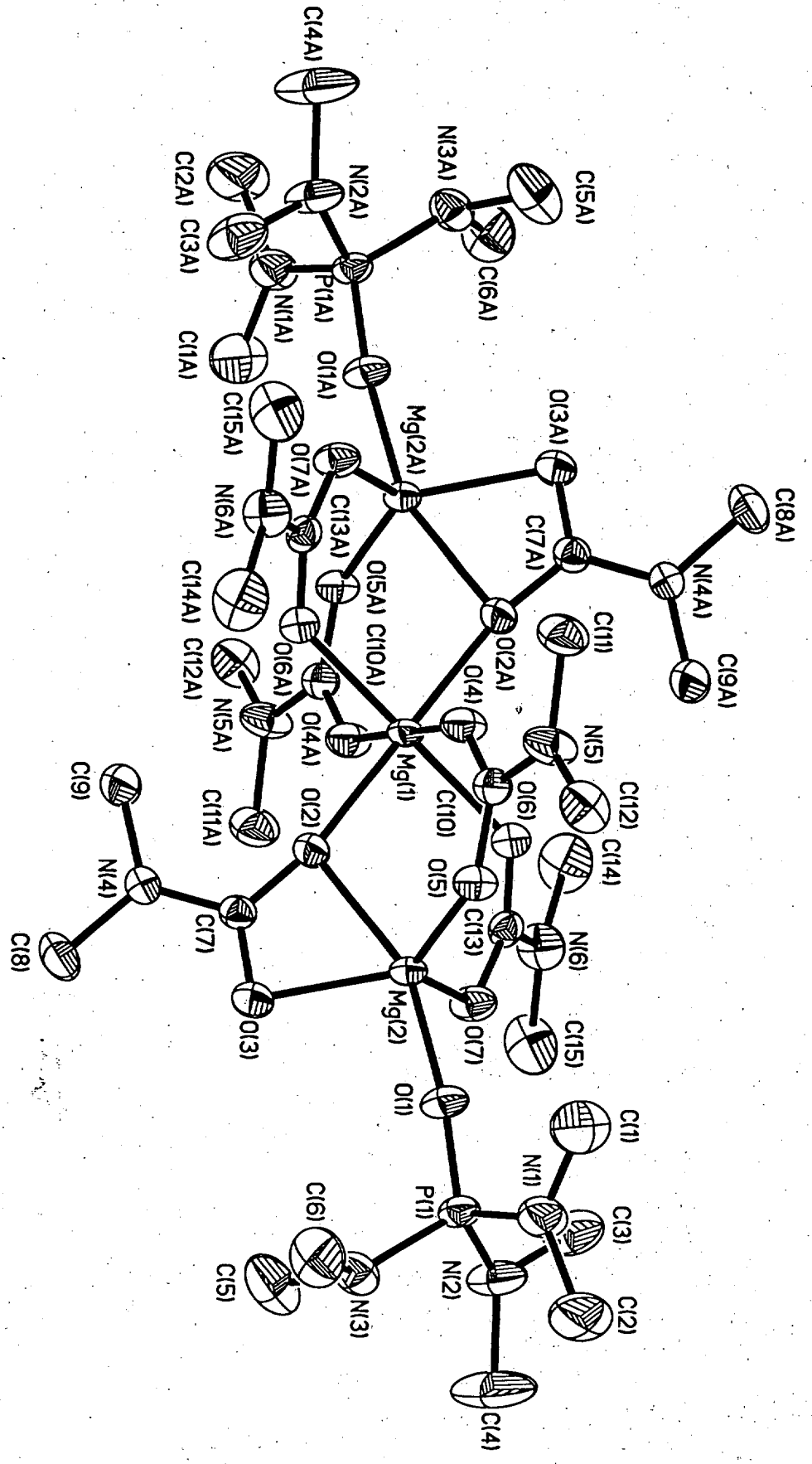


Fig. 1: The molecular structure of IC6413, thermal ellipsoids drawn at the 50% probability level.

Table 1. Crystal data and structure refinement for 6413.

Identification code	ic6413
Empirical formula	$C_{30}H_{72}Mg_3N_{12}O_{14}P_2$
Formula weight	959.87
Temperature	150(1) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 9.4391(3) Å alpha = 90° b = 11.0815(4) Å beta = 91.777(1)° c = 23.5656(8) Å gamma = 90°
Volume, Z	2463.8(2) $Å^3$, 2
Density (calculated)	1.294 Mg/m^3
Absorption coefficient	0.194 mm^{-1}
F(000)	1028
Crystal size	0.40 x 0.40 x 0.40 mm
θ range for data collection	1.73 to 26.38°
Limiting indices	$-11 \le h \le 11$, $-13 \le k \le 13$, $-29 \le l \le 20$
Reflections collected	12356
Independent reflections	5036 (R_{int} = 0.0258)
Absorption correction	empirical used sadabs
Max. and min. transmission	0.9280 and 0.8120
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5036 / 0 / 277
Goodness-of-fit on F^2	1.090
Final R indices [$I>2\sigma(I)$]	R1 = 0.0545, wR2 = 0.1534
R indices (all data)	R1 = 0.0659, wR2 = 0.1623
Largest diff. peak and hole	0.533 and -0.394 $eÅ^{-3}$

Table 2. Bond lengths [Å] and angles [°] for 6413.

Mg(1)-O(4)#1	2.033(2)	Mg(1)-O(4)	2.033(2)
Mg(1)-O(6)	2.045(2)	Mg(1)-O(6)#1	2.045(2)
Mg(1)-O(2)#1	2.094(2)	Mg(1)-O(2)	2.094(2)
Mg(1)-Mg(2)#1	3.4592(8)	Mg(1)-Mg(2)	3.4592(8)
Mg(2)-O(1)	1.967(2)	Mg(2)-O(5)	1.972(2)
Mg(2)-O(7)	1.988(2)	Mg(2)-O(3)	2.079(2)
Mg(2)-O(2)	2.179(2)	Mg(2)-C(7)	2.467(3)
Mg(2)-C(13)	2.794(3)	P(1)-O(1)	1.481(2)
P(1)-N(1)	1.630(3)	P(1)-N(2)	1.643(3)
P(1)-N(3)	1.644(2)	O(2)-C(7)	1.271(3)
O(3)-C(7)	1.267(3)	O(4)-C(10)	1.255(3)
O(5)-C(10)	1.278(3)	O(6)-C(13)	1.260(3)
O(7)-C(13)	1.272(3)	N(1)-C(1)	1.440(4)
N(1)-C(2)	1.463(4)	N(2)-C(3)	1.463(4)
N(2)-C(4)	1.468(4)	N(3)-C(6)	1.457(4)
N(3)-C(5)	1.471(4)	N(4)-C(7)	1.357(3)
N(4)-C(8)	1.443(3)	N(4)-C(9)	1.443(4)
N(5)-C(10)	1.374(3)	N(5)-C(12)	1.443(4)
N(5)-C(11)	1.449(4)	N(6)-C(13)	1.364(3)
N(6)-C(15)	1.441(4)	N(6)-C(14)	1.451(4)

O(4)#1-Mg(1)-O(4)	179.999(1)	O(4)#1-Mg(1)-O(6)	89.62(8)
O(4)-Mg(1)-O(6)	90.37(8)	O(4)#1-Mg(1)-O(6)#1	90.38(8)
O(4)-Mg(1)-O(6)#1	89.63(8)	O(6)-Mg(1)-O(6)#1	180.0
O(4)#1-Mg(1)-O(2)#1	87.95(8)	O(4)-Mg(1)-O(2)#1	92.05(8)
O(6)-Mg(1)-O(2)#1	92.10(7)	O(6)#1-Mg(1)-O(2)#1	87.90(7)
O(4)#1-Mg(1)-O(2)	92.05(8)	O(4)-Mg(1)-O(2)	87.95(8)
O(6)-Mg(1)-O(2)	87.90(7)	O(6)#1-Mg(1)-O(2)	92.10(7)
O(2)#1-Mg(1)-O(2)	180.000(1)	O(4)#1-Mg(1)-Mg(2)#1	69.15(5)
O(4)-Mg(1)-Mg(2)#1	110.85(5)	O(6)-Mg(1)-Mg(2)#1	121.84(6)
O(6)#1-Mg(1)-Mg(2)#1	58.16(6)	O(2)#1-Mg(1)-Mg(2)#1	36.78(5)
O(2)-Mg(1)-Mg(2)#1	143.22(5)	O(4)#1-Mg(1)-Mg(2)	110.85(5)
O(4)-Mg(1)-Mg(2)	69.15(5)	O(6)-Mg(1)-Mg(2)	58.16(6)
O(6)#1-Mg(1)-Mg(2)	121.84(6)	O(2)#1-Mg(1)-Mg(2)	143.22(5)
O(2)-Mg(1)-Mg(2)	36.78(5)	Mg(2)#1-Mg(1)-Mg(2)	180.0
O(1)-Mg(2)-O(5)	94.95(8)	O(1)-Mg(2)-O(7)	96.49(8)
O(5)-Mg(2)-O(7)	122.03(9)	O(1)-Mg(2)-O(3)	96.96(8)
O(5)-Mg(2)-O(3)	127.32(9)	O(7)-Mg(2)-O(3)	107.26(9)
O(1)-Mg(2)-O(2)	158.20(9)	O(5)-Mg(2)-O(2)	94.69(8)
O(7)-Mg(2)-O(2)	94.88(8)	O(3)-Mg(2)-O(2)	61.83(7)
O(1)-Mg(2)-C(7)	127.78(9)	O(5)-Mg(2)-C(7)	114.45(9)
O(7)-Mg(2)-C(7)	101.94(9)	O(3)-Mg(2)-C(7)	30.89(8)
O(2)-Mg(2)-C(7)	30.96(7)	O(1)-Mg(2)-C(13)	117.16(8)
O(5)-Mg(2)-C(13)	105.32(8)	O(7)-Mg(2)-C(13)	24.10(7)
O(3)-Mg(2)-C(13)	113.87(8)	O(2)-Mg(2)-C(13)	78.80(7)
C(7)-Mg(2)-C(13)	96.30(8)	O(1)-Mg(2)-Mg(1)	166.28(7)
O(5)-Mg(2)-Mg(1)	75.78(6)	O(7)-Mg(2)-Mg(1)	80.47(6)
O(3)-Mg(2)-Mg(1)	96.72(6)	O(2)-Mg(2)-Mg(1)	35.12(5)
C(7)-Mg(2)-Mg(1)	65.85(6)	C(13)-Mg(2)-Mg(1)	57.42(5)
O(1)-P(1)-N(1)	108.23(13)	O(1)-P(1)-N(2)	110.03(12)
N(1)-P(1)-N(2)	112.6(2)	O(1)-P(1)-N(3)	116.82(12)
N(1)-P(1)-N(3)	106.41(14)	N(2)-P(1)-N(3)	102.79(14)
P(1)-O(1)-Mg(2)	166.49(14)	C(7)-O(2)-Mg(1)	162.4(2)
C(7)-O(2)-Mg(2)	87.1(2)	Mg(1)-O(2)-Mg(2)	108.10(8)
C(7)-O(3)-Mg(2)	91.7(2)	C(10)-O(4)-Mg(1)	137.8(2)
C(10)-O(5)-Mg(2)	130.5(2)	C(13)-O(6)-Mg(1)	134.3(2)
C(13)-O(7)-Mg(2)	116.2(2)	C(1)-N(1)-C(2)	115.2(3)
C(1)-N(1)-P(1)	123.6(2)	C(2)-N(1)-P(1)	121.1(2)
C(3)-N(2)-C(4)	113.1(3)	C(3)-N(2)-P(1)	117.4(2)

C(4)-N(2)-P(1)	124.8(2)	C(6)-N(3)-C(5)	111.8(3)
C(6)-N(3)-P(1)	118.9(2)	C(5)-N(3)-P(1)	117.3(2)
C(7)-N(4)-C(8)	120.4(2)	C(7)-N(4)-C(9)	122.0(2)
C(8)-N(4)-C(9)	117.6(2)	C(10)-N(5)-C(12)	122.5(2)
C(10)-N(5)-C(11)	119.6(2)	C(12)-N(5)-C(11)	117.1(2)
C(13)-N(6)-C(15)	120.5(2)	C(13)-N(6)-C(14)	119.0(3)
C(15)-N(6)-C(14)	118.8(3)	O(3)-C(7)-O(2)	119.2(2)
O(3)-C(7)-N(4)	120.2(2)	O(2)-C(7)-N(4)	120.6(2)
O(3)-C(7)-Mg(2)	57.38(13)	O(2)-C(7)-Mg(2)	61.90(13)
N(4)-C(7)-Mg(2)	176.9(2)	O(4)-C(10)-O(5)	125.8(2)
O(4)-C(10)-N(5)	116.6(2)	O(5)-C(10)-N(5)	117.6(2)
O(6)-C(13)-O(7)	123.5(2)	O(6)-C(13)-N(6)	118.4(2)
O(7)-C(13)-N(6)	118.1(2)	O(6)-C(13)-Mg(2)	84.2(2)
O(7)-C(13)-Mg(2)	39.65(12)	N(6)-C(13)-Mg(2)	157.2(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1

Table 3. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 6413. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

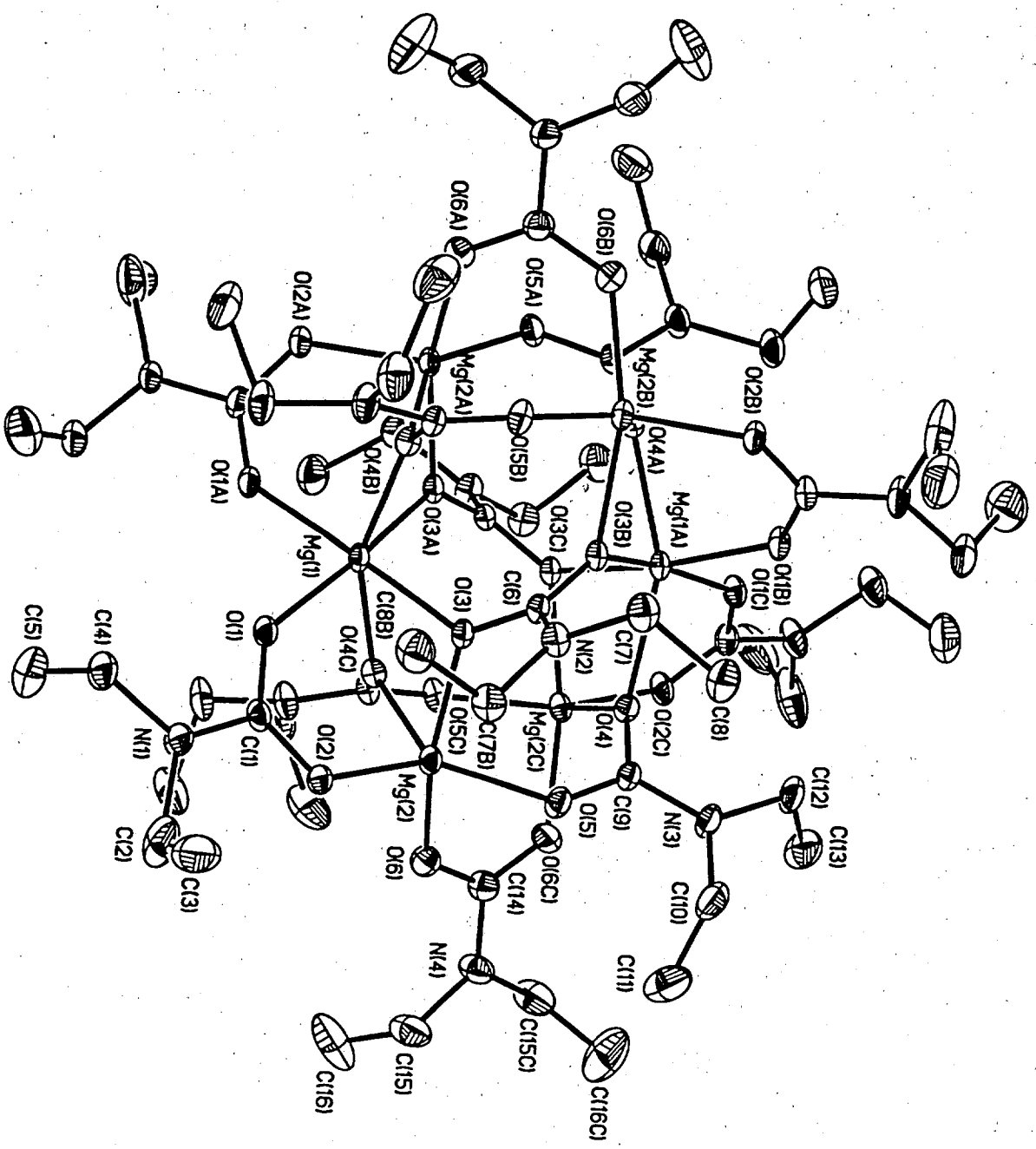
	x	y	z	U(eq)
Mg(1)	0	5000	5000	23(1)
Mg(2)	814(1)	5348(1)	3588(1)	22(1)
P(1)	1401(1)	5150(1)	2164(1)	26(1)
O(1)	941(2)	5236(2)	2758(1)	30(1)
O(2)	1057(2)	6120(2)	4436(1)	28(1)
O(3)	2161(2)	6819(2)	3702(1)	32(1)
O(4)	-1788(2)	5244(2)	4510(1)	31(1)
O(5)	-1275(2)	5353(2)	3583(1)	27(1)
O(6)	561(2)	3568(2)	4508(1)	32(1)
O(7)	1937(2)	3873(2)	3770(1)	30(1)
N(1)	13(3)	4857(3)	1759(1)	42(1)
N(2)	2645(3)	4122(3)	2115(1)	43(1)
N(3)	2145(3)	6356(2)	1897(1)	34(1)
N(4)	2625(2)	7672(2)	4565(1)	28(1)
N(5)	-3553(2)	5198(3)	3855(1)	36(1)
N(6)	2466(3)	2376(2)	4393(1)	36(1)
C(1)	-1416(4)	4876(4)	1955(2)	54(1)
C(2)	146(5)	4617(5)	1153(2)	76(2)
C(3)	2456(4)	2991(3)	2423(1)	50(1)
C(4)	3593(5)	4004(5)	1636(2)	80(2)
C(5)	3476(4)	6778(4)	2171(2)	60(1)
C(6)	1247(4)	7358(3)	1710(2)	54(1)
C(7)	1940(3)	6852(2)	4229(1)	23(1)
C(8)	3659(3)	8475(3)	4332(1)	43(1)
C(9)	2327(4)	7801(3)	5159(1)	43(1)
C(10)	-2130(3)	5274(2)	3992(1)	25(1)
C(11)	-4572(3)	5234(3)	4302(1)	41(1)
C(12)	-4104(3)	5293(3)	3278(1)	39(1)
C(13)	1629(3)	3320(2)	4222(1)	24(1)
C(14)	2249(5)	1833(3)	4944(1)	54(1)
C(15)	3750(3)	2105(3)	4103(2)	51(1)

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 6413. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Mg(1)	26(1)	28(1)	14(1)	-1(1)	5(1)	-4(1)
Mg(2)	24(1)	25(1)	16(1)	1(1)	4(1)	1(1)
P(1)	33(1)	27(1)	16(1)	1(1)	6(1)	3(1)
O(1)	36(1)	34(1)	18(1)	1(1)	5(1)	8(1)
O(2)	33(1)	31(1)	21(1)	-1(1)	5(1)	-10(1)
O(3)	39(1)	34(1)	22(1)	2(1)	7(1)	-7(1)
O(4)	27(1)	44(1)	23(1)	-1(1)	3(1)	-2(1)
O(5)	24(1)	36(1)	22(1)	1(1)	3(1)	-2(1)
O(6)	35(1)	33(1)	28(1)	-6(1)	9(1)	-6(1)
O(7)	37(1)	30(1)	22(1)	5(1)	6(1)	8(1)
N(1)	44(2)	61(2)	23(1)	-3(1)	2(1)	-15(1)
N(2)	55(2)	43(2)	32(1)	5(1)	19(1)	20(1)
N(3)	37(1)	36(1)	30(1)	7(1)	2(1)	-3(1)
N(4)	30(1)	27(1)	29(1)	-2(1)	5(1)	-7(1)
N(5)	22(1)	58(2)	30(1)	5(1)	3(1)	0(1)
N(6)	41(1)	32(1)	35(1)	10(1)	-1(1)	6(1)
C(1)	39(2)	77(3)	45(2)	-7(2)	-4(2)	-1(2)
C(2)	77(3)	124(4)	27(2)	-19(2)	6(2)	-41(3)
C(3)	70(2)	40(2)	40(2)	3(1)	11(2)	22(2)
C(4)	100(4)	83(3)	59(3)	12(2)	49(3)	43(3)
C(5)	49(2)	69(3)	61(2)	15(2)	-3(2)	-20(2)
C(6)	71(2)	37(2)	52(2)	15(2)	-1(2)	4(2)
C(7)	22(1)	23(1)	25(1)	1(1)	3(1)	2(1)
C(8)	44(2)	42(2)	44(2)	2(1)	6(1)	-20(1)
C(9)	50(2)	50(2)	31(2)	-10(1)	7(1)	-22(2)
C(10)	26(1)	24(1)	25(1)	1(1)	2(1)	2(1)
C(11)	27(1)	53(2)	45(2)	-3(2)	10(1)	-2(1)
C(12)	31(2)	48(2)	38(2)	8(1)	-8(1)	-3(1)
C(13)	29(1)	23(1)	19(1)	-1(1)	-1(1)	-1(1)
C(14)	82(3)	41(2)	38(2)	16(2)	-10(2)	2(2)
C(15)	37(2)	38(2)	77(3)	7(2)	1(2)	11(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 6413.

	x	y	z	U(eq)
H(1A)	-1401(4)	5042(4)	2364(2)	80
H(1B)	-1864(4)	4091(4)	1882(2)	80
H(1C)	-1956(4)	5508(4)	1754(2)	80
H(2A)	1150(5)	4620(5)	1058(2)	114
H(2B)	-357(5)	5242(5)	932(2)	114
H(2C)	-265(5)	3826(5)	1061(2)	114
H(3A)	1816(4)	3125(3)	2737(1)	75
H(3B)	3376(4)	2710(3)	2575(1)	75
H(3C)	2049(4)	2382(3)	2165(1)	75
H(4A)	3680(5)	4786(5)	1446(2)	120
H(4B)	3202(5)	3410(5)	1366(2)	120
H(4C)	4530(5)	3737(5)	1776(2)	120
H(5A)	4051(4)	6081(4)	2291(2)	89
H(5B)	3262(4)	7269(4)	2504(2)	89
H(5C)	4002(4)	7265(4)	1902(2)	89
H(6A)	374(4)	7043(3)	1529(2)	80
H(6B)	1752(4)	7851(3)	1436(2)	80
H(6C)	1012(4)	7855(3)	2038(2)	80
H(8A)	4046(3)	9002(3)	4632(1)	65
H(8B)	3207(3)	8967(3)	4032(1)	65
H(8C)	4428(3)	8000(3)	4172(1)	65
H(9A)	2929(4)	8437(3)	5326(1)	65
H(9B)	2522(4)	7037(3)	5356(1)	65
H(9C)	1329(4)	8018(3)	5199(1)	65
H(11A)	-5533(3)	5170(3)	4135(1)	62
H(11B)	-4475(3)	5997(3)	4510(1)	62
H(11C)	-4396(3)	4559(3)	4563(1)	62
H(12A)	-5138(3)	5215(3)	3274(1)	59
H(12B)	-3701(3)	4649(3)	3048(1)	59
H(12C)	-3846(3)	6079(3)	3121(1)	59
H(14A)	2925(5)	1171(3)	5005(1)	81
H(14B)	1280(5)	1518(3)	4957(1)	81
H(14C)	2395(5)	2442(3)	5241(1)	81
H(15A)	4214(3)	1404(3)	4281(2)	76
H(15B)	4389(3)	2802(3)	4127(2)	76
H(15C)	3521(3)	1926(3)	3703(2)	76


O(6A)
O(6B)
O(2A)
O(5A)
Mg(2A)
Mg(2B)
O(2B)
O(4A)
O(1A)
O(4B)
O(5B)
O(3C)
O(3B)
Mg(1A)
Mg(1)
O(3A)
O(1B)
O(1C)
C(6)
O(3)
C(8B)
O(1)
C(5)
C(4)
O(4C)
N(2)
C(7)
C(8)
O(5C)
C(7B)
Mg(2C)
O(4)
O(2C)
N(1)
C(1)
O(2)
Mg(2)
O(5)
C(9)
N(3)
C(12)
C(13)
C(2)
C(3)
O(6)
O(6C)
C(14)
C(10)
C(11)
N(4)
C(15C)
C(15)
C(16)
C(16C)

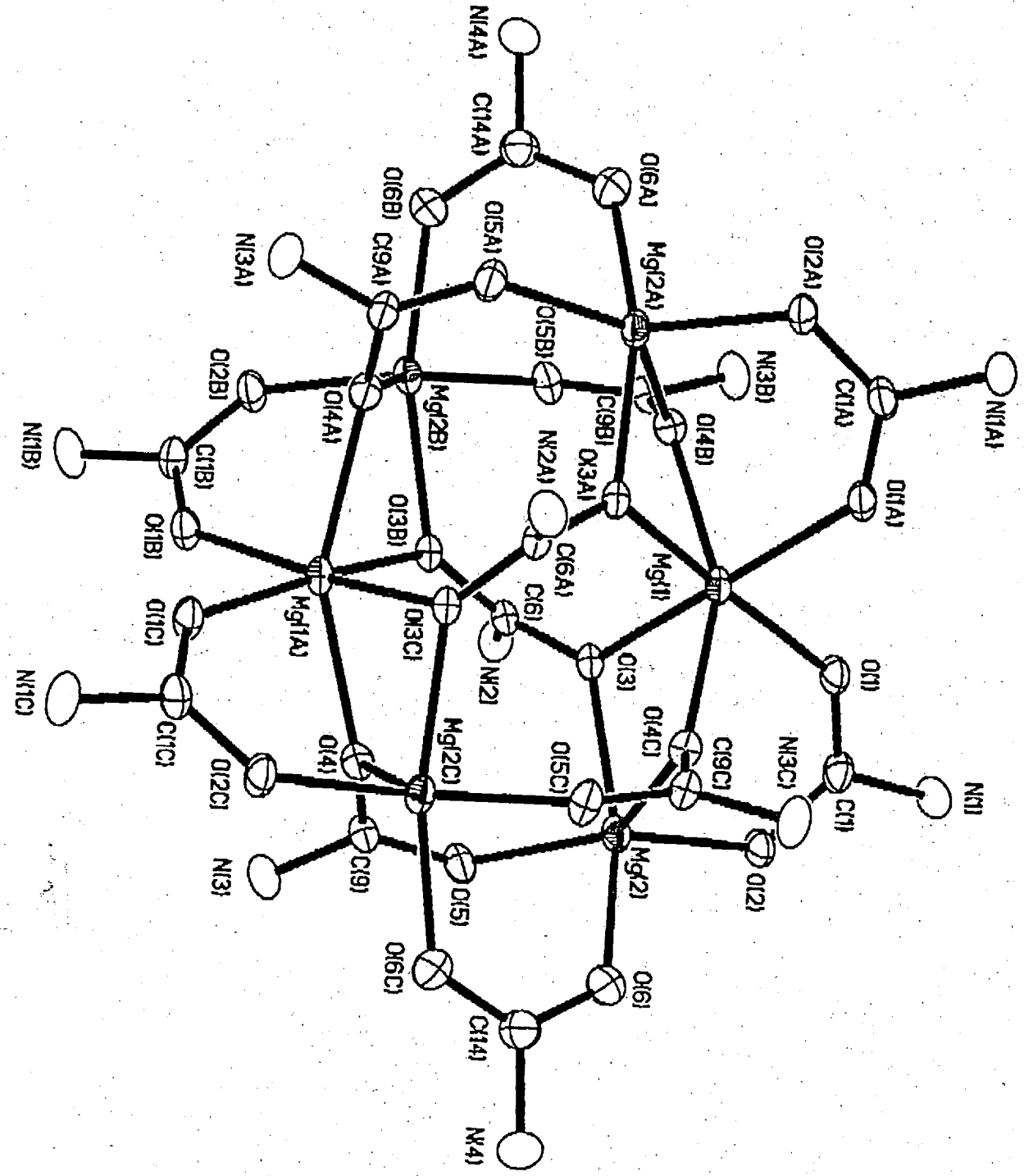


Table 1. Crystal data and structure refinement for 5464.

Identification code	ic5464
Empirical formula	$C_{60}H_{120}Mg_6N_{12}O_{24}$
Formula weight	1539.54
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Ccca
Unit cell dimensions	a = 20.9480(3) Å alpha = 90° b = 25.1843(1) Å beta = 90° c = 16.2816(1) Å gamma = 90°
Volume, Z	8589.53(14) $Å^3$, 4
Density (calculated)	1.191 Mg/m^3
Absorption coefficient	0.129 mm^{-1}
F(000)	3312
Crystal size	0.50 x 0.40 x 0.30 mm
θ range for data collection	1.62 to 25.02°
Limiting indices	$-24 \le h \le 12$, $-29 \le k \le 29$, $-19 \le l \le 18$
Reflections collected	17120
Independent reflections	3806 (R_{int} = 0.1124)
Absorption correction	Sadabs
Max. and min. transmission	0.9281 and 0.1053
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3806 / 0 / 234
Goodness-of-fit on F^2	0.953
Final R indices [I>2σ(I)]	R1 = 0.0566, wR2 = 0.1593
R indices (all data)	R1 = 0.1054, wR2 = 0.1850
Extinction coefficient	0.0007(2)
Largest diff. peak and hole	0.320 and -0.271 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 5464. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Mg(1)	5000	1615(1)	7500	60(1)
Mg(2)	3716(1)	2028(1)	6760(1)	66(1)
O(1)	4633(1)	1034(1)	6786(1)	74(1)
O(2)	3723(1)	1335(1)	6208(1)	77(1)
O(3)	4700(1)	2132(1)	6578(1)	61(1)
O(4)	4038(1)	3201(1)	7106(1)	67(1)
O(5)	3607(1)	2702(1)	6119(1)	78(1)
O(6)	2831(1)	2103(1)	7184(2)	93(1)
N(1)	4066(2)	505(1)	5958(2)	108(1)
N(2)	5000	2500	5375(2)	75(1)
N(3)	3518(2)	3582(1)	6032(2)	92(1)
N(4)	1903(2)	2500	7500	102(2)
C(1)	4147(2)	982(1)	6337(2)	76(1)
C(2)	3471(5)	398(3)	5483(4)	194(4)
C(3)	3629(4)	517(3)	4676(6)	248(6)
C(4)	4512(2)	63(2)	6088(3)	123(2)
C(5)	4308(3)	-290(2)	6756(5)	200(3)
C(6)	5000	2500	6192(3)	61(1)
C(7)	5334(2)	2910(2)	4907(2)	95(1)
C(8)	4923(3)	3368(2)	4690(3)	137(2)
C(9)	3726(2)	3148(1)	6428(2)	68(1)
C(10)	3152(3)	3522(2)	5262(3)	134(2)
C(11)	2502(3)	3324(2)	5368(4)	172(3)
C(12)	3618(2)	4118(2)	6384(3)	118(2)
C(13)	3060(3)	4308(2)	6875(4)	156(2)
C(14)	2549(2)	2500	7500	82(1)
C(15)	1553(2)	2080(2)	7089(4)	139(2)
C(16)	1288(4)	1690(3)	7617(5)	252(5)

Table 3. Bond lengths [Å] and angles [°] for 5464.

Mg(1)-O(1)#1	2.021(2)	Mg(1)-O(1)	2.021(2)
Mg(1)-O(3)	2.084(2)	Mg(1)-O(3)#1	2.084(2)
Mg(1)-O(4)#2	2.165(2)	Mg(1)-O(4)#3	2.165(2)
Mg(1)-Mg(2)#1	3.1257(11)	Mg(1)-Mg(2)	3.1257(11)
Mg(2)-O(2)	1.963(2)	Mg(2)-O(6)	1.987(3)
Mg(2)-O(5)	2.005(2)	Mg(2)-O(4)#3	2.049(2)
Mg(2)-O(3)	2.100(2)	Mg(2)-C(1)	2.870(3)
Mg(2)-Mg(2)#3	3.385(2)	O(1)-C(1)	1.261(4)
O(2)-C(1)	1.275(4)	O(3)-C(6)	1.283(3)
O(4)-C(9)	1.289(4)	O(4)-Mg(2)#3	2.049(2)
O(4)-Mg(1)#2	2.165(2)	O(5)-C(9)	1.256(4)
O(6)-C(14)	1.271(3)	N(1)-C(1)	1.360(4)
N(1)-C(4)	1.468(5)	N(1)-C(2)	1.491(8)
N(2)-C(6)	1.331(5)	N(2)-C(7)#2	1.462(4)
N(2)-C(7)	1.462(4)	N(3)-C(9)	1.343(4)
N(3)-C(10)	1.476(5)	N(3)-C(12)	1.480(5)
N(4)-C(14)	1.353(6)	N(4)-C(15)#3	1.452(5)
N(4)-C(15)	1.452(5)	C(2)-C(3)	1.388(12)
C(4)-C(5)	1.469(7)	C(6)-O(3)#2	1.283(3)
C(7)-C(8)	1.481(6)	C(10)-C(11)	1.461(8)
C(12)-C(13)	1.496(7)	C(14)-O(6)#3	1.271(3)
C(15)-C(16)	1.417(8)		

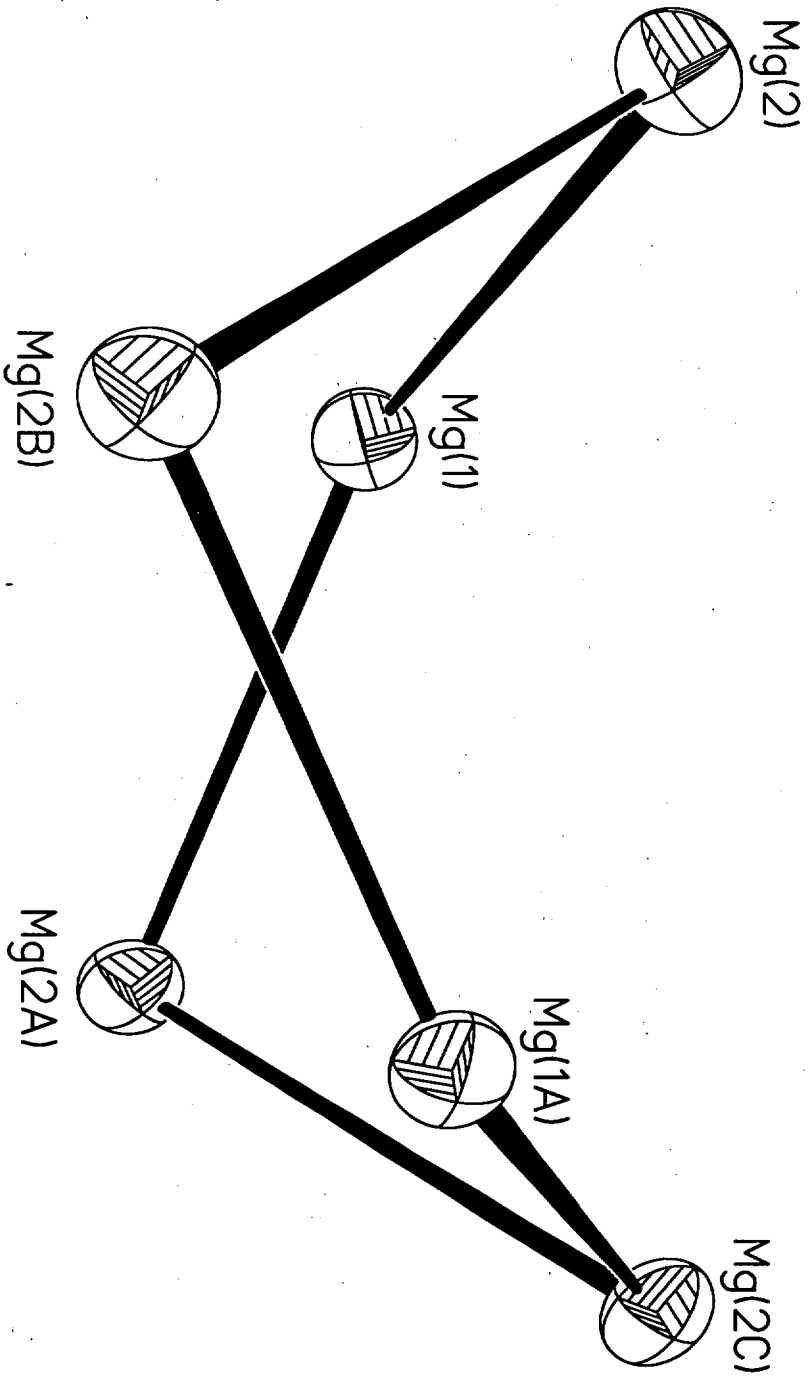
O(1)#1-Mg(1)-O(1)	87.15(13)	O(1)#1-Mg(1)-O(3)	168.95(9)
O(1)-Mg(1)-O(3)	85.65(8)	O(1)#1-Mg(1)-O(3)#1	85.65(8)
O(1)-Mg(1)-O(3)#1	168.94(9)	O(3)-Mg(1)-O(3)#1	102.64(11)
O(1)#1-Mg(1)-O(4)#2	88.38(8)	O(1)-Mg(1)-O(4)#2	109.76(9)
O(3)-Mg(1)-O(4)#2	86.18(8)	O(3)#1-Mg(1)-O(4)#2	78.43(8)
O(1)#1-Mg(1)-O(4)#3	109.76(9)	O(1)-Mg(1)-O(4)#3	88.38(8)
O(3)-Mg(1)-O(4)#3	78.43(8)	O(3)#1-Mg(1)-O(4)#3	86.18(8)
O(4)#2-Mg(1)-O(4)#3	155.31(12)	O(1)#1-Mg(1)-Mg(2)#1	72.08(6)
O(1)-Mg(1)-Mg(2)#1	142.16(7)	O(3)-Mg(1)-Mg(2)#1	109.21(7)
O(3)#1-Mg(1)-Mg(2)#1	41.85(6)	O(4)#2-Mg(1)-Mg(2)#1	40.72(6)
O(4)#3-Mg(1)-Mg(2)#1	128.00(6)	O(1)#1-Mg(1)-Mg(2)	142.16(7)
O(1)-Mg(1)-Mg(2)	72.08(6)	O(3)-Mg(1)-Mg(2)	41.85(6)
O(3)#1-Mg(1)-Mg(2)	109.21(7)	O(4)#2-Mg(1)-Mg(2)	128.01(6)
O(4)#3-Mg(1)-Mg(2)	40.71(6)	Mg(2)#1-Mg(1)-Mg(2)	141.14(5)
O(2)-Mg(2)-O(6)	104.46(11)	O(2)-Mg(2)-O(5)	121.01(11)
O(6)-Mg(2)-O(5)	89.69(10)	O(2)-Mg(2)-O(4)#3	99.19(10)
O(6)-Mg(2)-O(4)#3	91.18(11)	O(5)-Mg(2)-O(4)#3	138.14(10)
O(2)-Mg(2)-O(3)	92.27(9)	O(6)-Mg(2)-O(3)	162.43(10)
O(5)-Mg(2)-O(3)	86.16(9)	O(4)#3-Mg(2)-O(3)	80.72(9)
O(2)-Mg(2)-C(1)	21.79(9)	O(6)-Mg(2)-C(1)	117.62(11)
O(5)-Mg(2)-C(1)	133.50(11)	O(4)#3-Mg(2)-C(1)	81.60(10)
O(3)-Mg(2)-C(1)	76.82(9)	O(2)-Mg(2)-Mg(1)	82.79(7)
O(6)-Mg(2)-Mg(1)	134.45(9)	O(5)-Mg(2)-Mg(1)	125.47(8)
O(4)#3-Mg(2)-Mg(1)	43.57(6)	O(3)-Mg(2)-Mg(1)	41.47(6)
C(1)-Mg(2)-Mg(1)	61.06(8)	O(2)-Mg(2)-Mg(2)#3	161.83(10)
O(6)-Mg(2)-Mg(2)#3	71.71(8)	O(5)-Mg(2)-Mg(2)#3	77.07(7)
O(4)#3-Mg(2)-Mg(2)#3	63.64(6)	O(3)-Mg(2)-Mg(2)#3	90.72(6)
C(1)-Mg(2)-Mg(2)#3	144.65(9)	Mg(1)-Mg(2)-Mg(2)#3	87.65(3)
C(1)-O(1)-Mg(1)	135.7(2)	C(1)-O(2)-Mg(2)	123.4(2)
C(6)-O(3)-Mg(1)	131.0(2)	C(6)-O(3)-Mg(2)	129.77(13)
Mg(1)-O(3)-Mg(2)	96.68(9)	C(9)-O(4)-Mg(2)#3	125.1(2)
C(9)-O(4)-Mg(1)#2	138.4(2)	Mg(2)#3-O(4)-Mg(1)#2	95.72(9)
C(9)-O(5)-Mg(2)	121.7(2)	C(14)-O(6)-Mg(2)	130.5(3)
C(1)-N(1)-C(4)	121.6(3)	C(1)-N(1)-C(2)	119.9(4)
C(4)-N(1)-C(2)	118.0(4)	C(6)-N(2)-C(7)#2	121.4(3)

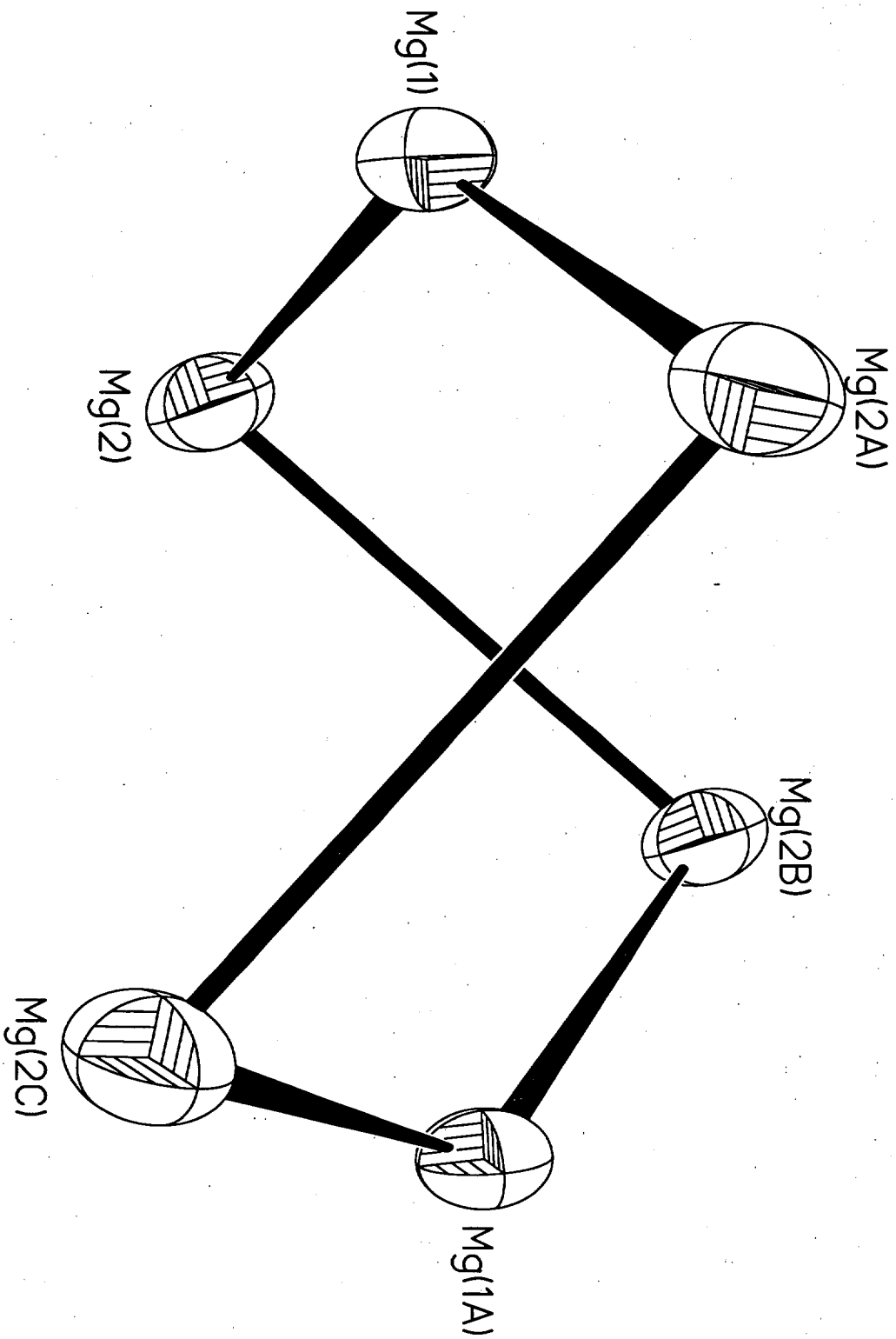
C(9)-N(3)-C(10)	119.5(3)	C(9)-N(3)-C(12)	120.7(3)
C(10)-N(3)-C(12)	119.7(3)	C(14)-N(4)-C(15)#3	120.3(2)
C(14)-N(4)-C(15)	120.3(2)	C(15)#3-N(4)-C(15)	119.3(5)
O(1)-C(1)-O(2)	125.9(3)	O(1)-C(1)-N(1)	117.1(3)
O(2)-C(1)-N(1)	117.0(3)	O(1)-C(1)-Mg(2)	91.1(2)
O(2)-C(1)-Mg(2)	34.83(13)	N(1)-C(1)-Mg(2)	151.6(3)
C(3)-C(2)-N(1)	104.7(8)	N(1)-C(4)-C(5)	112.3(5)
O(3)#2-C(6)-O(3)	121.3(4)	O(3)#2-C(6)-N(2)	119.4(2)
O(3)-C(6)-N(2)	119.3(2)	N(2)-C(7)-C(8)	113.4(3)
O(5)-C(9)-O(4)	122.5(3)	O(5)-C(9)-N(3)	118.1(3)
O(4)-C(9)-N(3)	119.4(3)	C(11)-C(10)-N(3)	114.8(5)
N(3)-C(12)-C(13)	112.8(4)	O(6)-C(14)-O(6)#3	124.6(5)
O(6)-C(14)-N(4)	117.7(2)	O(6)#3-C(14)-N(4)	117.7(2)
C(16)-C(15)-N(4)	115.0(5)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+3/2 #2 -x+1,-y+1/2,z #3 x+1-1,-y+1/2,-z+3/2

IC5464




Mg(1)
Mg(2)
Mg(2A)
Mg(2B)
Mg(2C)
Mg(1A)

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ENVIRONMENT OF MG1

Ligand	Symcode	Dist.	Angles			
MG1A	1555	4.457				
MG2	1555	3.126	70.6			
MG2B	1555	4.512	40.8	99.1		
MG2A	1555	3.126	70.6	141.1	48.5	
MG2C	1555	4.512	40.8	48.5	81.6	99.1

ENVIRONMENT OF MG2

Ligand	Symcode	Dist.	Angles			
MG1	1555	3.126				
MG1A	1555	4.513	68.6			
MG2B	1555	5.882	49.2	31.6		
MG2A	1555	5.895	19.4	49.2	33.4	
MG2C	1555	3.385	87.7	43.8	73.5	73.1

ENVIRONMENT OF MG2A

Ligand	Symcode	Dist.	Angles			
MG1	1555	3.126				
MG1A	1555	4.512	68.6			
MG2	1555	5.895	19.4	49.2		
MG2B	1555	3.385	87.7	43.8	73.1	
MG2C	1555	5.882	49.2	31.6	33.4	73.5

ENVIRONMENT OF MG1A

Ligand	Symcode	Dist.	Angles			
MG1	1555	4.457				
MG2	1555	4.513	40.8			
MG2B	1555	3.126	70.6	99.1		
MG2A	1555	4.512	40.8	81.6	48.5	
MG2C	1555	3.126	70.6	48.5	141.1	99.1

ENVIRONMENT OF MG2B

Ligand	Symcode	Dist.	Angles			
MG1	1555	4.512				
MG1A	1555	3.126	68.6			
MG2	1555	5.882	31.6	49.2		
MG2A	1555	3.385	43.8	87.7	73.5	
MG2C	1555	5.895	49.2	19.4	33.4	73.1

ENVIRONMENT OF MG2C

Ligand	Symcode	Dist.	Angles			
MG1	1555	4.512				
MG1A	1555	3.126	68.6			
MG2	1555	3.385	43.8	87.7		
MG2B	1555	5.895	49.2	19.4	73.1	

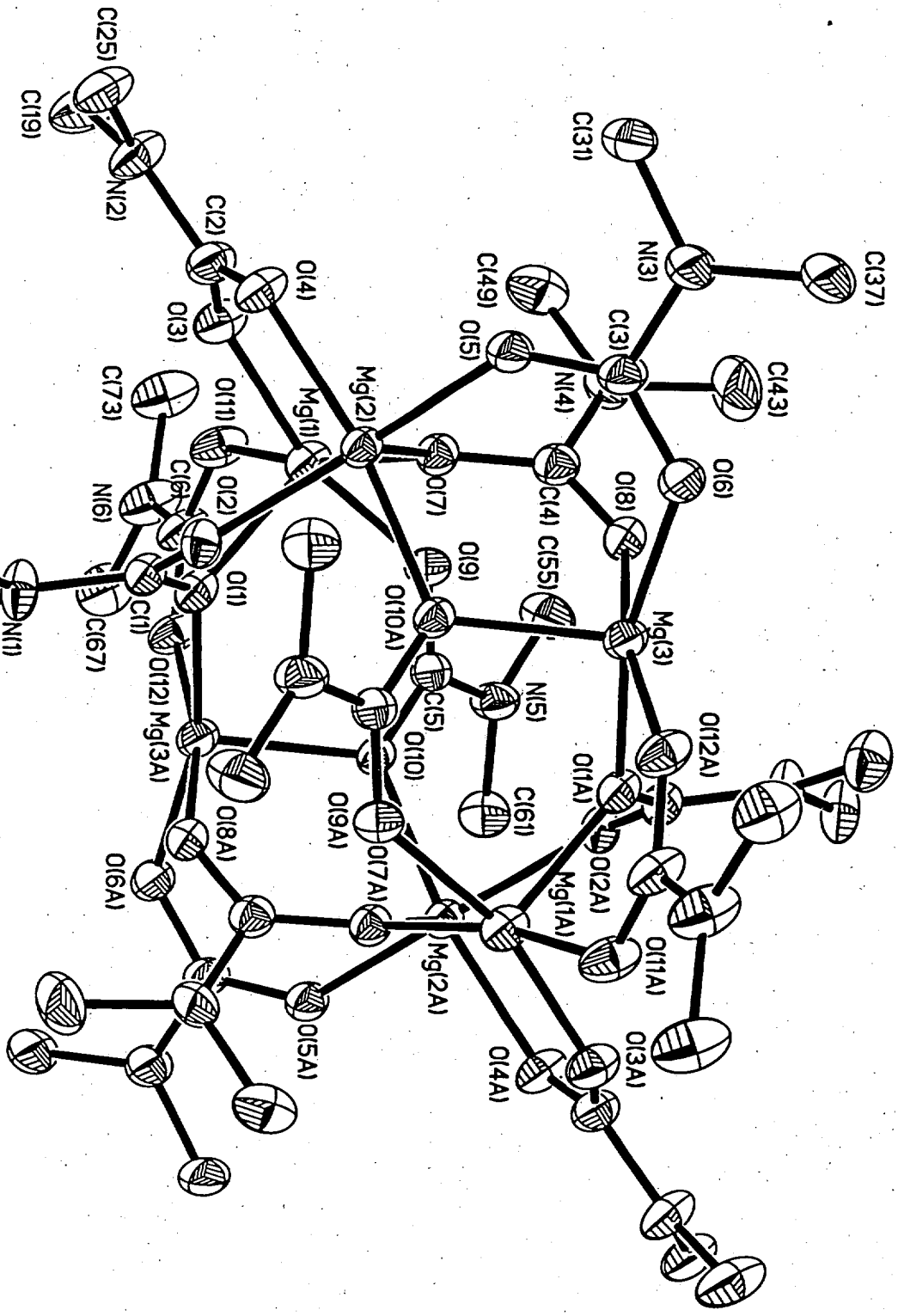

Fig. 1: The molecular structure of IC6360, thermal ellipsoids drawn at the 30% probability level.

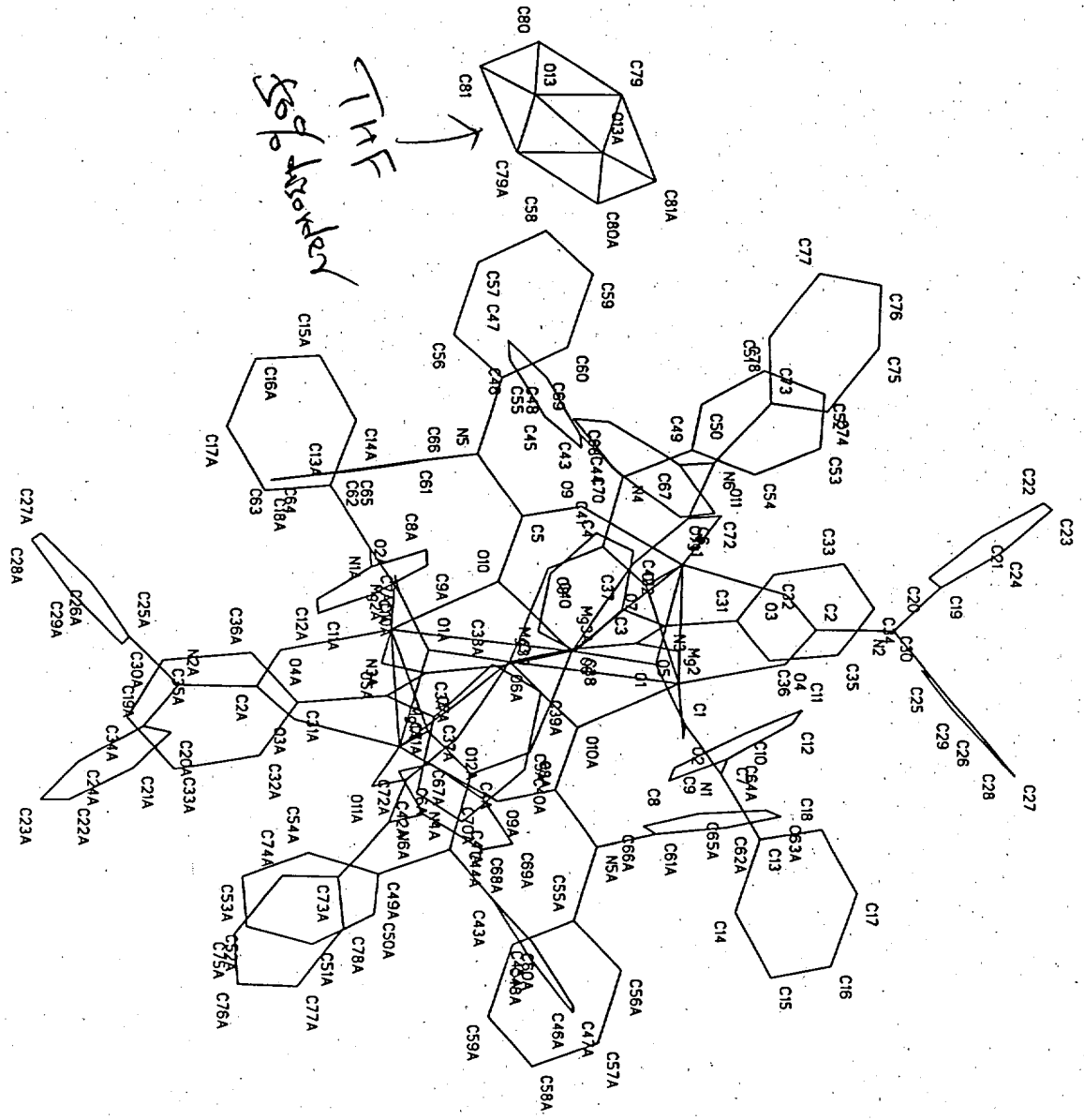

Table 1. Crystal data and structure refinement for 6360.

Identification code	ic6360
Empirical formula	$C_{160}H_{128}Mg_6N_{12}O_{25}$
Formula weight	2764.60
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 15.4528(6) Å alpha = 103.826(1)°
	b = 15.5306(6) Å beta = 103.406(1)°
	c = 16.7324(6) Å gamma = 109.074(1)°
Volume, Z	3468.7(2) $Å^3$, 1
Density (calculated)	1.323 Mg/m^3
Absorption coefficient	0.114 mm^{-1}
F(000)	1444
Crystal size	0.74 x 0.40 x 0.15 mm
θ range for data collection	1.33 to 25.00°
Limiting indices	$-19 \le h \le 19$, $-15 \le k \le 19$, $-20 \le l \le 20$
Reflections collected	27391
Independent reflections	11906 (R_{int} = 0.0361)
Absorption correction	empirical used sadabs
Max. and min. transmission	0.9280 and 0.7639
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11216 / 0 / 909
Goodness-of-fit on F^2	1.062
Final R indices [I>2σ(I)]	R1 = 0.0990, wR2 = 0.2721
R indices (all data)	R1 = 0.1422, wR2 = 0.3111
Extinction coefficient	0.015(2)
Largest diff. peak and hole	0.991 and -0.531 $eÅ^{-3}$

Table 2. Bond lengths [Å] and angles [°] for 6360.

Mg(1)-O(11)	1.993(3)	Mg(1)-O(3)	1.998(4)
Mg(1)-O(1)	2.040(4)	Mg(1)-O(9)	2.046(3)
Mg(1)-O(7)	2.054(3)	Mg(1)-Mg(3)#1	3.377(2)
Mg(1)-Mg(2)	3.415(2)	Mg(2)-O(5)	2.000(3)
Mg(2)-O(4)	2.008(3)	Mg(2)-O(7)	2.042(3)
Mg(2)-O(2)	2.046(3)	Mg(2)-O(10)#1	2.074(3)
Mg(2)-Mg(3)	3.417(2)	Mg(3)-O(6)	1.989(3)
Mg(3)-O(12)#1	2.008(3)	Mg(3)-O(10)#1	2.032(3)
Mg(3)-O(8)	2.053(4)	Mg(3)-O(1)#1	2.054(3)
Mg(3)-Mg(1)#1	3.377(2)	O(1)-C(1)	1.286(5)
O(1)-Mg(3)#1	2.054(3)	O(2)-C(1)	1.235(5)
O(3)-C(2)	1.240(6)	O(4)-C(2)	1.262(6)
O(5)-C(3)	1.256(5)	O(6)-C(3)	1.253(5)
O(7)-C(4)	1.287(5)	O(8)-C(4)	1.234(5)
O(9)-C(5)	1.249(5)	O(10)-C(5)	1.282(5)
O(10)-Mg(3)#1	2.032(3)	O(10)-Mg(2)#1	2.074(3)
O(11)-C(6)	1.255(6)	O(12)-C(6)	1.248(6)
O(12)-Mg(3)#1	2.008(3)	N(1)-C(1)	1.367(6)
N(1)-C(13)	1.418(7)	N(1)-C(7)	1.456(7)
N(2)-C(2)	1.404(6)	N(2)-C(19)	1.434(7)
N(2)-C(25)	1.444(7)	N(3)-C(3)	1.401(6)
N(3)-C(37)	1.439(7)	N(3)-C(31)	1.443(7)
N(4)-C(4)	1.366(6)	N(4)-C(49)	1.422(7)
N(4)-C(43)	1.434(8)	N(5)-C(5)	1.353(6)
N(5)-C(55)	1.437(7)	N(5)-C(61)	1.464(6)
N(6)-C(6)	1.401(6)	N(6)-C(73)	1.424(8)
N(6)-C(67)	1.437(7)	C(7)-C(12)	1.345(9)
C(7)-C(8)	1.364(8)	C(8)-C(9)	1.360(9)
C(9)-C(10)	1.379(11)	C(10)-C(11)	1.357(11)
C(11)-C(12)	1.349(10)	C(13)-C(14)	1.372(10)
C(13)-C(18)	1.378(9)	C(14)-C(15)	1.385(11)
C(15)-C(16)	1.372(13)	C(16)-C(17)	1.396(13)
C(17)-C(18)	1.393(11)	C(19)-C(20)	1.345(9)
C(19)-C(24)	1.357(10)	C(20)-C(21)	1.391(10)
C(21)-C(22)	1.361(14)	C(22)-C(23)	1.36(2)
C(23)-C(24)	1.370(12)	C(25)-C(30)	1.352(8)
C(25)-C(26)	1.361(9)	C(26)-C(27)	1.381(12)
C(27)-C(28)	1.339(12)	C(28)-C(29)	1.355(11)
C(29)-C(30)	1.391(9)	C(31)-C(36)	1.330(12)
C(31)-C(32)	1.336(13)	C(32)-C(33)	1.413(12)
C(33)-C(34)	1.39(3)	C(34)-C(35)	1.33(2)
C(35)-C(36)	1.401(14)	C(37)-C(38)	1.365(9)
C(37)-C(42)	1.370(10)	C(38)-C(39)	1.411(9)
C(39)-C(40)	1.362(12)	C(40)-C(41)	1.358(12)
C(41)-C(42)	1.378(10)	C(43)-C(48)	1.27(2)
C(43)-C(44)	1.355(14)	C(44)-C(45)	1.34(2)
C(45)-C(46)	1.35(4)	C(46)-C(47)	1.31(5)
C(47)-C(48)	1.45(2)	C(49)-C(50)	1.346(10)
C(49)-C(54)	1.362(10)	C(50)-C(51)	1.318(13)
C(51)-C(52)	1.32(2)	C(52)-C(53)	1.325(13)
C(53)-C(54)	1.366(10)	C(55)-C(60)	1.352(9)
C(55)-C(56)	1.405(9)	C(56)-C(57)	1.396(13)
C(57)-C(58)	1.401(14)	C(58)-C(59)	1.391(14)
C(59)-C(60)	1.398(11)	C(61)-C(66)	1.369(9)
C(61)-C(62)	1.391(8)	C(62)-C(63)	1.358(9)
C(63)-C(64)	1.373(11)	C(64)-C(65)	1.400(12)
C(65)-C(66)	1.375(10)	C(67)-C(68)	1.351(11)
C(67)-C(72)	1.351(10)	C(68)-C(69)	1.406(13)
C(69)-C(70)	1.41(2)	C(70)-C(71)	1.31(2)

C(71)-C(72)	1.383(13)	C(73)-C(78)	1.221(13)
C(73)-C(74)	1.265(12)	C(74)-C(75)	1.41(2)
C(75)-C(76)	1.190(14)	C(76)-C(77)	1.31(2)
C(77)-C(78)	1.42(2)	O(13)-C(81)	1.14(3)
O(13)-C(80)	1.31(3)	O(13)-C(79)#2	1.38(3)
O(13)-C(79)	1.62(3)	O(13)-O(13)#2	1.73(5)
C(79)-O(13)#2	1.38(3)	C(79)-C(80)	1.87(4)
C(79)-C(81)#2	2.02(4)	C(80)-C(81)	1.33(4)
C(81)-C(79)#2	2.02(4)		

O(11)-Mg(1)-O(3)	91.78(14)	O(11)-Mg(1)-O(1)	94.2(2)
O(3)-Mg(1)-O(1)	95.8(2)	O(11)-Mg(1)-O(9)	87.9(2)
O(3)-Mg(1)-O(9)	164.1(2)	O(1)-Mg(1)-O(9)	100.06(13)
O(11)-Mg(1)-O(7)	165.6(2)	O(3)-Mg(1)-O(7)	89.62(13)
O(1)-Mg(1)-O(7)	99.88(13)	O(9)-Mg(1)-O(7)	86.83(13)
O(11)-Mg(1)-Mg(3)#1	77.76(11)	O(3)-Mg(1)-Mg(3)#1	126.01(12)
O(1)-Mg(1)-Mg(3)#1	34.55(9)	O(9)-Mg(1)-Mg(3)#1	69.41(10)
O(7)-Mg(1)-Mg(3)#1	112.68(10)	O(11)-Mg(1)-Mg(2)	157.18(13)
O(3)-Mg(1)-Mg(2)	68.98(11)	O(1)-Mg(1)-Mg(2)	76.40(10)
O(9)-Mg(1)-Mg(2)	113.96(10)	O(7)-Mg(1)-Mg(2)	33.39(9)
Mg(3)#1-Mg(1)-Mg(2)	103.16(5)	O(5)-Mg(2)-O(4)	93.40(14)
O(5)-Mg(2)-O(7)	94.45(14)	O(4)-Mg(2)-O(7)	94.10(14)
O(5)-Mg(2)-O(2)	168.1(2)	O(4)-Mg(2)-O(2)	87.02(14)
O(7)-Mg(2)-O(2)	97.38(13)	O(5)-Mg(2)-O(10)#1	91.06(12)
O(4)-Mg(2)-O(10)#1	166.4(2)	O(7)-Mg(2)-O(10)#1	98.38(12)
O(2)-Mg(2)-O(10)#1	85.98(12)	O(5)-Mg(2)-Mg(1)	123.50(12)
O(4)-Mg(2)-Mg(1)	76.65(10)	O(7)-Mg(2)-Mg(1)	33.61(8)
O(2)-Mg(2)-Mg(1)	68.16(10)	O(10)#1-Mg(2)-Mg(1)	111.33(9)
O(5)-Mg(2)-Mg(3)	68.65(9)	O(4)-Mg(2)-Mg(3)	158.44(12)
O(7)-Mg(2)-Mg(3)	76.21(9)	O(2)-Mg(2)-Mg(3)	113.04(10)
O(10)#1-Mg(2)-Mg(3)	33.27(8)	Mg(1)-Mg(2)-Mg(3)	102.76(5)
O(6)-Mg(3)-O(12)#1	93.7(2)	O(6)-Mg(3)-O(10)#1	95.83(13)
O(12)#1-Mg(3)-O(10)#1	94.53(14)	O(6)-Mg(3)-O(8)	87.67(14)
O(12)#1-Mg(3)-O(8)	168.1(2)	O(10)#1-Mg(3)-O(8)	97.12(13)
O(6)-Mg(3)-O(1)#1	163.5(2)	O(12)#1-Mg(3)-O(1)#1	90.30(13)
O(10)#1-Mg(3)-O(1)#1	99.87(13)	O(8)-Mg(3)-O(1)#1	85.24(14)
O(6)-Mg(3)-Mg(1)#1	159.23(13)	O(12)#1-Mg(3)-Mg(1)#1	68.62(10)
O(10)#1-Mg(3)-Mg(1)#1	75.69(9)	O(8)-Mg(3)-Mg(1)#1	111.95(11)
O(1)#1-Mg(3)-Mg(1)#1	34.30(10)	O(6)-Mg(3)-Mg(2)	76.89(10)
O(12)#1-Mg(3)-Mg(2)	123.36(12)	O(10)#1-Mg(3)-Mg(2)	34.05(8)
O(8)-Mg(3)-Mg(2)	68.47(9)	O(1)#1-Mg(3)-Mg(2)	114.00(10)
Mg(1)#1-Mg(3)-Mg(2)	103.28(5)	C(1)-O(1)-Mg(1)	118.4(3)
C(1)-O(1)-Mg(3)#1	130.0(3)	Mg(1)-O(1)-Mg(3)#1	111.2(2)
C(1)-O(2)-Mg(2)	137.6(3)	C(2)-O(3)-Mg(1)	139.4(3)
C(2)-O(4)-Mg(2)	126.7(3)	C(3)-O(5)-Mg(2)	138.8(3)
C(3)-O(6)-Mg(3)	126.8(3)	C(4)-O(7)-Mg(2)	119.3(3)
C(4)-O(7)-Mg(1)	127.4(3)	Mg(2)-O(7)-Mg(1)	113.00(14)
C(4)-O(8)-Mg(3)	137.3(3)	C(5)-O(9)-Mg(1)	135.3(3)
C(5)-O(10)-Mg(3)#1	118.8(3)	C(5)-O(10)-Mg(2)#1	128.5(3)
Mg(3)#1-O(10)-Mg(2)#1	112.68(14)	C(6)-O(11)-Mg(1)	125.1(3)
C(6)-O(12)-Mg(3)#1	138.8(3)	C(1)-N(1)-C(13)	119.9(4)
C(1)-N(1)-C(7)	121.4(4)	C(13)-N(1)-C(7)	118.5(4)
C(2)-N(2)-C(19)	122.6(5)	C(2)-N(2)-C(25)	120.6(4)
C(19)-N(2)-C(25)	116.7(4)	C(3)-N(3)-C(37)	121.5(4)
C(3)-N(3)-C(31)	121.0(4)	C(37)-N(3)-C(31)	117.5(4)
C(4)-N(4)-C(49)	121.4(4)	C(4)-N(4)-C(43)	118.5(4)
C(49)-N(4)-C(43)	119.2(4)	C(5)-N(5)-C(55)	121.7(4)
C(5)-N(5)-C(61)	120.1(4)	C(55)-N(5)-C(61)	116.2(4)
C(6)-N(6)-C(73)	123.0(5)	C(6)-N(6)-C(67)	118.8(5)
C(73)-N(6)-C(67)	118.1(4)	O(2)-C(1)-O(1)	124.9(4)
O(2)-C(1)-N(1)	119.4(4)	O(1)-C(1)-N(1)	115.7(4)
O(3)-C(2)-O(4)	127.5(4)	O(3)-C(2)-N(2)	117.5(4)
O(4)-C(2)-N(2)	115.0(5)	O(6)-C(3)-O(5)	127.6(4)